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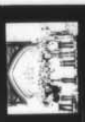

ATOMIC SCATTERING THEORY

MATHEMATICAL and COMPUTATIONAL ASPECTS

Proceedings of a conference held at
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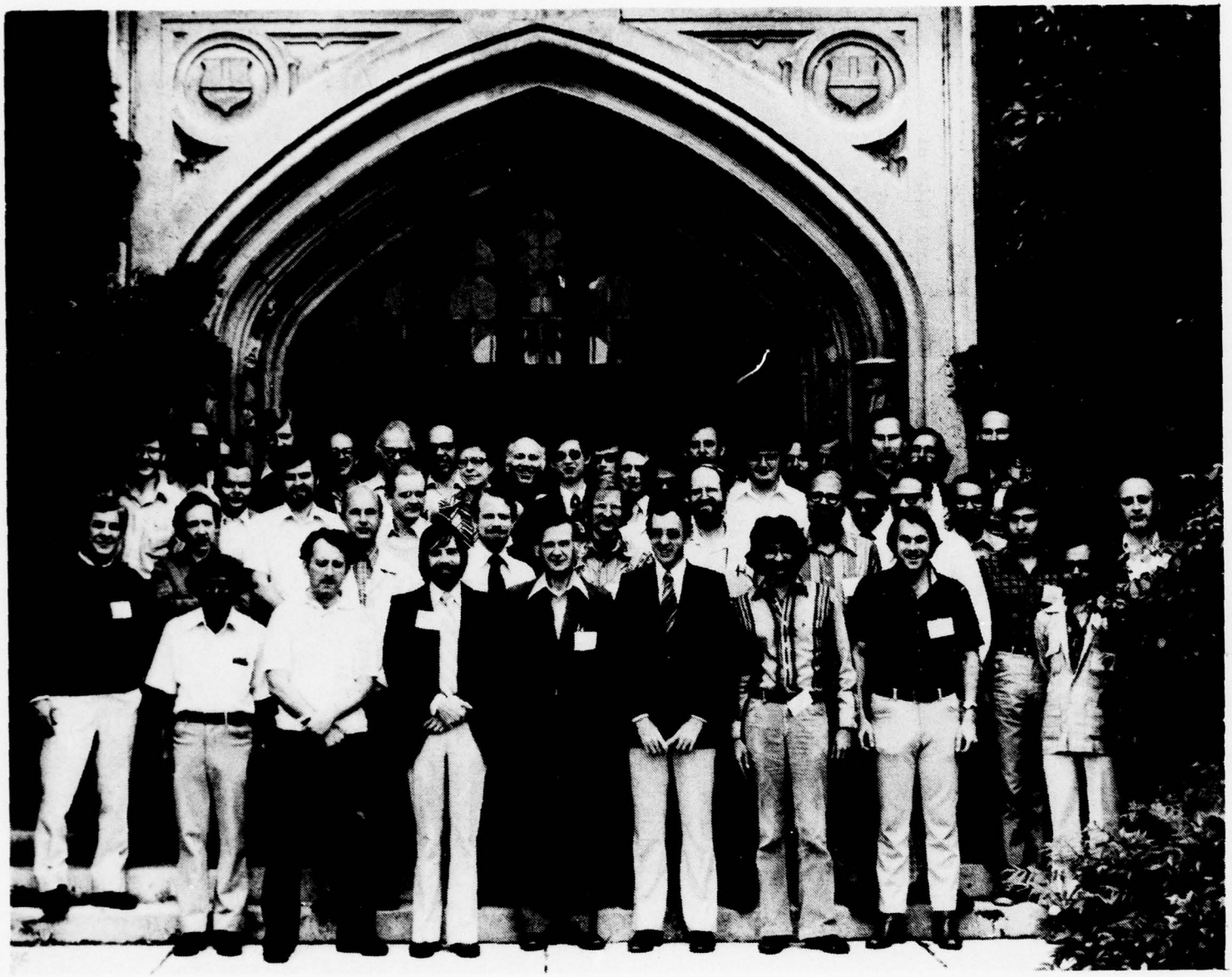

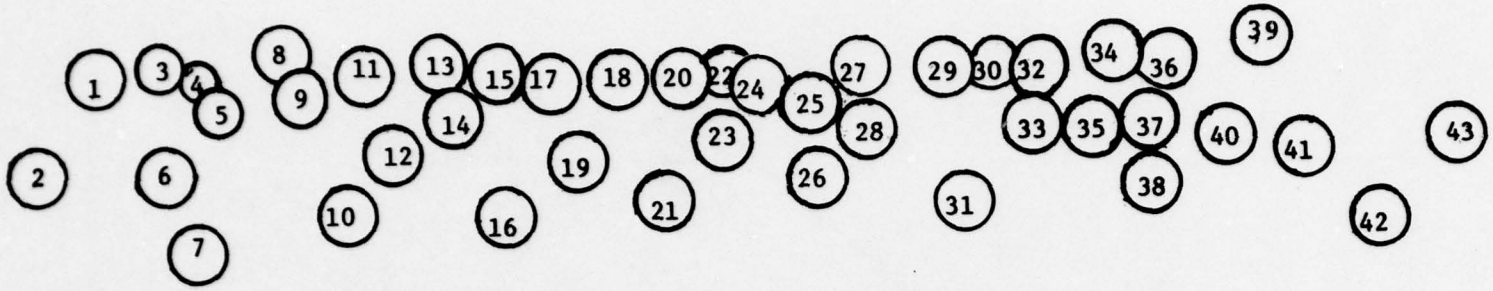

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Preface

This volume presents the proceedings of the Conference on Mathematical and Computational Aspects of Atomic Scattering Theory, which was held June 7-9, 1978 at the University of Western Ontario. About 50 scientists participated in the meeting, which was organized by T.M. Luke and J. Nuttall of the Theoretical Physics Group of the University of Western Ontario.

The aim of the conference was to bring together people who approach the problems of Atomic Scattering Theory from varying viewpoints, which range from the rigorous mathematical to the purely computational. Ten invited speakers gave lectures which appear in full in the following pages. Summaries of the contributions of other participants follow.

The organizers wish to express their appreciation for the generous financial support which made the conference possible. The agencies who helped were IBM Canada Ltd., National Research Council Canada, the U.S. Air Force Office of Scientific Research, the U.S. Navy Office of Naval Research and the University of Western Ontario. Many people at the University of Western Ontario helped with the arrangements for the conference, and to all of them we are most grateful. In particular, the support and encouragement of Dr. W.P. Alford, Chairman of the Physics Department, was most valuable. Mrs. Marion Anderson carried out the secretarial work with constant cheerfulness and efficiency. A special touch at refreshment time was provided by a group of faculty wives. Finally we thank all those who participated in the meeting, and hope they will return to see us another day.

AN OVERVIEW OF RIGOROUS SCATTERING THEORY

B. Simon

We discuss the three main foundational problems of rigorous scattering theory: existence of wave operators, completeness of wave operators and absence of singular spectrum. We describe many of the mathematical techniques: Cook's method, the trace class theory of Kato and Birman, Kato's theory of smooth perturbations, the weighted L^2 method of Agmon and Kuroda and the new approach of V. Enss.

1 Introduction

The bulk of the rigorous work in scattering theory has concerned itself with three main problems; we begin by describing them in the simplest situation where $H = H_o + V$ with $H_o = -\Delta$ and V "short range", e.g. e^{-r}/r.

(a) Existence of Wave Operators We generally describe a prepared state in terms of parameters most suitable for a particle moving under the influence of H_o. Thus, if $e^{-itH_o}\phi$ is a free wave packet (think of ϕ as peaked about certain momenta), one wants an interacting wave packet, $e^{-itH}\psi$ so that

$$\| e^{-itH_o}\phi - e^{-itH}\psi \| \to 0 \text{ as } t \to -\infty . \tag{1.1}$$

Since e^{itH} is unitary

$$\psi = \lim_{t \to -\infty} e^{itH} e^{-itH_o}\phi . \tag{1.2}$$

If we deal only with physical (i.e. normalizable) states, we expect that the limit in (1.2) will exist for all ϕ in the basic Hilbert space of the problem, $L^2(R^3)$. In that case, the limit is said to exist in the strong operator topology and we write

$$\Omega^{\pm}(H,H_o) = \text{s-}\lim_{t \to \pm\infty} e^{itH} e^{-itH_o} . \tag{1.3}$$

$\Omega^{\pm}$ are called the wave operators and the first problem is to show that the limit in (1.3) exists. We note that the strange convention on the $\pm$ in (1.3) is standard in the physics literature although it is only sometimes used in the more mathematical literature. It comes from the fact that $\Omega^{\pm}$ is connected with the resolvent $R(z) = (z - H)^{-1}$ for $z = x \pm i0$ (with x real) in the time-independent theory. Also note that since $e^{itH} e^{-itH_0}$ is unitary

$$\| \Omega^{\pm} \phi \| = \| \phi \| \quad . \tag{1.4}$$

(b) Completeness of Wave Operators It is a standard argument in quantum mechanics courses that unitarity of the S-matrix is merely an expression of conservation of probability. There is a hidden additional assumption that is being made here. After all, S is given by the condition that $|(\eta, S\phi)|^2$ is just the probability that a state which looks like $e^{-itH_0} \phi$ in the distant past and which moves under e^{-itH} will look like $e^{-itH_0} \eta$ in the distant future, i.e. $(\eta, S\phi)$ is the overlap of $\Omega^{+}\phi$ and $\Omega^{-}\eta$ which leads to

$$S = (\Omega^{-})^{*} \Omega^{+} \quad . \tag{1.5}$$

(1.4) immediately tells us how $(\Omega^{\pm})^{*}$ operate. They must be the inverse of $\Omega^{\pm}$ on $\mathrm{Ran}(\Omega^{\pm})$ since $(\Omega^{+})^{*} \Omega^{+} = (\Omega^{-})^{*} \Omega^{-} = 1$ (by (1.4)). But suppose that $\eta \perp \mathrm{Ran}\ \Omega^{+}$. Then $(\eta, \Omega^{+}\phi) = 0$ for all ϕ so that $(\Omega^{+})^{*}\eta \perp$ all ϕ so $(\Omega^{+})^{*}\eta = 0$. Thus $(\Omega^{+})^{*}$ is 0 on $(\mathrm{Ran}\ \Omega^{+})^{\perp}$ and the inverse of Ω^{+} on $\mathrm{Ran}\ \Omega^{+}$. This means that S preserves norms only if $\mathrm{Ran}\ \Omega^{+} \subset \mathrm{Ran}\ \Omega^{-}$. Similarly S^{*} preserves norms only if $\mathrm{Ran}\ \Omega^{-} \subset \mathrm{Ran}\ \Omega^{+}$. Thus $S^{*}S = SS^{*} = 1$ if and only if

$$\mathrm{Ran}\ \Omega^{+} = \mathrm{Ran}\ \Omega^{-} \quad . \tag{1.6}$$

Proving (1.6) is sometimes called the problem of weak asymptotic completeness. Physically, it corresponds to the assertion that any state which is asymptotically free in the past will also be of that type in the future; it is clear that such an assumption is tacitly made in deducing unitarity of S from "conservation of

probability". How can (1.6) fail? It's not easy, but Pearson [22] has constructed a singular potential V so that $H = -\Delta + V$ is well-defined and physically reasonably (i.e. self-adjoint and bounded from below) and so that $\Omega^{\pm}$ exist but with (1.6) false! For his H, one can take a vector $\phi = \Omega^{+}\eta$ so that as $t \to +\infty$, $e^{-itH}\phi$ breaks into two pieces, one of which moves out to infinity; the other asymptotically approaches 0 which is where V is very singular. Often, one asks about a stronger property than (1.6), namely that

$$\text{Ran } \Omega^{+} = \text{Ran } \Omega^{-} = \mathcal{H}_{pp}^{\perp} \tag{1.7}$$

where $\mathcal{H}_{pp}$ is the span of the eigenvectors of H. Physically (1.7), which is called <u>asymptotic completeness</u> asserts that any state is either bound (in $\mathcal{H}_{pp}$) or a scattering state (in Ran Ω^{+} = Ran Ω^{-}); here, "either" is intended in the quantum mechanical sense, that is, we mean any state is a superposition of a bound and a scattering state.

(c) <u>Absence of Singular Continuous Spectrum</u> To describe the last problem requires a very short course in functional analysis; for a more detailed "course", see [25]. If H is any self-adjoint operator and ϕ is any vector, there is a measure $d\mu$ on $(-\infty, \infty)$ so that $(\phi, e^{-itH}\phi) = \int e^{-itx}\, d\mu(x)$. $d\mu$ is called the <u>spectral measure</u> (of ϕ, for H). To understand the kind of pathology about which one can worry, we need to consider a measure constructed by Cantor. First, Cantor constructed a function, f, as follows: $f = 0$ on $(-\infty, 0]$, $f = 1$ on $[1, \infty)$; f is only interesting on (0,1) where it is given by $f = \frac{1}{2}$ on (1/3, 2/3); $f = 1/4$ on (1/9, 2/9) and 3/4 on (7/9), 8/9), $f = 1/8$ on (1/27, 2/27) etc. Formally if $x = \sum_{n=1}^{\infty} a_n/3^n$ with each $a_n = 0,1,2$, then let N(x) = first n with $a_{n+1} = 1$ (N = ∞ if each $a_n = 0$ or 2) and

$$f(x) = 1/2 + \sum_{n=1}^{N(x)} (a_n - 1)/2^{n+1}$$

Notice that f is a queer function indeed: it is continuous and at any x with $N(x) < \infty$, f is differentiable with $f'(x) = 0$. The set of such points has size $1/3 + 2(1/9) + 4(1/27) + \ldots = 1$ but f is not constant! The *Cantor measure* is the Lebesgue Stieltjes measure df determined by f. Thus, for nice g, one can define $\int g\, df$ as one does the Riemann integral by $\lim_{n\to\infty} \sum_{k=1}^{2^n} g(k/2^n)$ $[f(k/2^n) - f((k-1)/2^n)]$. The Cantor measure has no pure points, i.e. $\lim_{\varepsilon\to 0} \int_{a-\varepsilon}^{a+\varepsilon} df = 0$ for all a but it still manages to live on a set of Lebesgue measure 1-1 = 0. Such a pathological measure is called a singular continuous measure. The Lebesgue decomposition theorem asserts that any measure has the form $d\mu = d\mu_{pp} + d\mu_{ac} + d\mu_{sing}$ where $d\mu_{pp}$ is pure point, literally of the form $\sum_{n=1}^{\infty} a_n \delta(x-x_n)$, $d\mu_{ac}$ is of the form $g(x)dx$ and $d\mu_{sing}$ is singular continuous. Using this result, one shows that given any self-adjoint operator H on a Hilbert space $\mathcal{H}$, there is a decomposition $\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sing}$ so that $\phi \in \mathcal{H}_{pp}$ (etc.) if and only if the spectral measure of ϕ for H is pure point (etc.). The last problem of the three is to prove that

$$\mathcal{H}_{sing} = \{0\} . \tag{1.8}$$

Why should we expect this? $\mathcal{H}_{pp}$ is precisely the span of the eigenvectors of H. Moreover, we claim that

$$\mathcal{H}_{ac} \supset \text{Ran } \Omega^{\pm} \tag{1.9}$$

so that (1.7) is equivalent to the pair of statements: (1.8) and

$$\text{Ran } \Omega^{+} = \text{Ran } \Omega^{-} = \mathcal{H}_{ac} . \tag{1.10}$$

(1.10) is often called completeness. To prove (1.9), we note that

$$e^{isH}\, \Omega^{\pm}\, e^{-isH_0} = \underset{t \to \pm\infty}{\text{s-lim}}\; e^{i(s+t)H}\, e^{-i(s+t)H_0} = \Omega^{\pm} ,$$

so

$$e^{isH}\,\Omega^{\pm} = \Omega^{\pm}\,e^{isH_o}\ , \tag{1.11}$$

and thus $(\Omega^{+}\phi,\ e^{isH}\,\Omega^{+}\phi) = (\phi,\ e^{isH_o}\,\phi)$. This says that the spectral measure of $\Omega^{+}\phi$ for H is the same as that of ϕ for H_o; this is just a sophisticated form of conservation of energy. Since $H_o = -\Delta$ has purely absolutely continuous spectrum, (1.9) holds.

Pearson [23] has announced results on the existence of potentials V on $(-\infty, \infty)$ with V smooth and $V(x) \to 0$ at infinity so that $-\frac{d^2}{dx^2} + V$ has only singular continuous spectrum. It is worthwhile describing his example in some detail since it illustrates the kind of dynamical behavior that occurs when H has singular spectrum. Let V be an even function on $(-\infty, \infty)$, so that for x positive,

$$V(x) = \sum_{n=0}^{\infty} a_n\, f(x - y_n)\ ,$$

where f is a fixed non-negative C^{∞} function with support in $(-\frac{1}{2},\frac{1}{2})$, the a_n's obey $\Sigma a_n^{\,2} = \infty$ (but this can be done with $a_n \to 0$) and the y_n's are given by the condition

$$y_{n+1} - y_n = \exp(e^n)\ .$$

Pearson's statement is that for this V we have purely singular spectrum. Rather than try to describe his proof, let us give his argument as to why physically one expects the result. The canonical example of a potential which manages to have absolutely continuous states without V going to zero is a periodic potential with its Bloch wave packets. The particle manages to get through the infinity of bumps by cleverly building up coherences, i.e. the phases necessary for it to get through one bump help it get through the next. In this case, the enormous separation between y's causes the particle to "forget" any coherence it has built up; one can

imagine the particle as successively undergoing independent collisions with potentials $a_n f$. By the Born approximation, for a_n small, the reflection from this potential is $O(a_n^2)$. The condition $\Sigma a_n^2 = \infty$ implies no particles reach infinity. Moreover, by tunnelling, the positivity of V and the inability to build up coherence, one expects no bound states. Thus, particles moving under H wander aimlessly about and this is precisely what corresponds to singular spectrum. Indeed, if $f(t) \equiv (\phi, e^{-itH}\phi) = \int e^{-ixt}\, d\mu(x)$ with $d\mu$ singular continuous, then f goes to zero in some average sense, since a theorem of Wiener assures that for the Fourier transform of any continuous measure:

$$\frac{1}{2T}\int_{-T}^{T} |f(t)|^2\, dt \to 0 \tag{1.12}$$

On the other hand, f may not go to zero pointwise; for example, for the Cantor measure,

$$f(t) = e^{-\frac{1}{2}it} \prod_{n=1}^{\infty} \cos(3^{-n} t)\ ,$$

so that $|f(2\pi 3^m)| = |f(2\pi)| \neq 0$ for all m. This can only happen for singular measures; if μ is absolutely continuous, then the Riemann-Lebesgue lemma asserts that $f(t) \to 0$ as $t \to \infty$.

This completes our description of the three basic problems of rigorous scattering theory. In the rest of this paper, we will give a quick hit-and-run description of most of the major techniques of the subject. The one technique that we leave out is that of "complex scaling" or "dilation analyticity" - in part because it is not very scattering theoretic and, in part, because the proceedings of the March 1978 Sanibel Workshop [29] give a comprehensive overview of much of the subject. We also concentrate on the two body case with $r^{-1-\varepsilon}$ potentials where things are easier to describe. However, we should mention that wave operators in multiparticle situations had to be extended to consider channel

wave operators: a channel, α, of a N-body system, is a decomposition, $D(\alpha)$, of the particles into disjoint clusters $C_1,\ldots,C_k$ and bound states $\eta_1,\ldots,\eta_k$ of the Hamiltonian $H(C_i)$ of the internal motion of the clusters. One defines $H_D = H - I_D$ where H is the Hamiltonian of the whole system with center of mass motion removed and I_D is the sum of all potentials between particles in different clusters. Also one lets P_α be the projection onto all states of the form $(\Pi\eta_i)\phi$ with ϕ a function of the differences of the centers of mass of the cluster. Then, the channel wave operator is

$$\Omega_\alpha^{\pm} = \underset{t \to \mp\infty}{\text{s-lim}}\ e^{itH} e^{-itH_\alpha} P_\alpha \tag{1.13}$$

A result of Jauch [15] asserts that if one is careful about counting channels associated with degenerate eigenvalues of $H(C_i)$, then the Ran Ω_α^+ are mutually orthogonal. Asymptotic completeness then says that

$$\bigoplus_\alpha \text{Ran}\ \Omega_\alpha^+ = \bigoplus_\alpha \text{Ran}\ \Omega_\alpha^- = \mathcal{H}_{pp}^{\perp} \tag{1.14}$$

We should also mention that for $V = \lambda|r|^{-1}$, the s-lim (1.3) does not exist [8] because of the celebrated infinite phases of the Coulomb scattering problem. Rather one needs a modified dynamics, $U_D(t) = \exp(-if(-i\nabla,t))$, so chosen that

$$\Omega_D^{\pm} = \underset{t \to \mp\infty}{\text{s-lim}}\ e^{itH} U_D(t)$$

exists but so that (1.11) is still true (this will happen so long as $f(-i\nabla, t + s) - f(-i\nabla,t) \to s(-\Delta)$ as $t \to \infty$ with s fixed, e.g. $f(-i\nabla, t) = t(-\Delta) + t^\alpha g(\Delta)$ or $+ (\ell n(t)g(\Delta))$. The proper physics will occur if $\int [|e^{-itH_0}\phi| - |U_D(t)\phi|]^2 \to 0$ so that up to "unimportant phases", $e^{-itH}\Omega_D^+\eta$ looks like $e^{-itH_0}\eta$ as $t \to -\infty$.

For a more detailed review of the status of the problems and more exhaustive presentation of the methods, see [26,27]. We note here that problem (a) has been solved in extremely great generality and the problems (b) and (c) for the two body case have also been solved. For the N-body case, problems (b) and (c) have only been solved in some special cases at the present instant (e.g. 3-bodies, or repulsive potentials, or weak coupling or "generic" dilation analytic potentials with sufficient fall off). However, Enss [10] is very close to extending his method described in Section 6 to N bodies and Combes [5] has a program based on the method of weighted L^2-space (Section 5) and some ideas of Deift-Simon [7], which appears promising. I hope that these problems will be solved soon and will free our energies for studying some of the more physical problems in the subject.

Finally I should attempt to explain why a practicing atomic theorist should care about the work on these questions which after all involve issues where any betting man would wager a great deal on the truth of the "obvious" answers. Let me give some reasons:

(a) Atomic physics should be a science and not an art: in studying a model like the purely Coulombic Hamiltonian, one should be able to derive basic properties like the unitarity of the S-matrix from first principles even if the derivation is not easy.

(b) These studies occasionally provide new insights into or even unexpected theorems about issues of direct experimental interest. I might mention, somewhat immodestly, my own theorem [30] concerning the absence of resonances in atomic systems at energies sufficient to <u>completely</u> ionize the atom.

(c) Occasionally, new calculational tools come from the rigorous work. The canonical example would be the famous work of Faddeev: he was motivated by wishing to solve the three basic problems we have described but his work has produced a computational industry!

"Rigorous" and "practical" atomic physics are two fields which have not interacted much with each other. Recently, there has been some attempts to change this and I regard this development as very exciting. The possibilities for cross-pollinization are very great indeed.

2 Cook's Method [6]

In virtually all Hilbert space theoretic scattering problems including optical and acoustical scattering as well as non-relativistic quantum scattering, one can solve the wave operator existence by a general method known as Cook's method or by one of its variants. One first notes that by a simple density argument (the $\varepsilon/3$ trick [25]), it suffices to prove that the limit (1.2) exists for a dense set of ϕ. Indeed, since $e^{+itH}\, e^{-itH_o}$ is linear, it need only be proven for a <u>total set</u>, i.e. a set whose finite linear combinations is dense. Using the completeness of a Hilbert space, we see that:

PROPOSITION 2.1 <u>Let</u> $W(t) \equiv e^{+itH}\, e^{-itH_o}$. <u>In order for the limit (1.2) to exist for all</u> ϕ, <u>it suffices that there is a total set</u> $\mathfrak{D}$ <u>so that for any</u> $\phi \in \mathfrak{D}$:

$$\lim_{t,s \to \pm \infty} \| [W(t) - W(s)]\, \phi \| = 0$$

How can we estimate $(W(t) - W(s))\, \phi$? Simple. Suppose that $W(t)\phi$ is differentiable. Then, for $s < t$

$$\| [W(t) - W(s)]\, \phi \| \leq \int_s^t \| \frac{d}{du} W(u)\, \phi \|\, du \tag{2.1}$$

by the fundamental theorem of calculus. Moreover if $H = H_o + V$, then, at least formally

$$\frac{d}{dt}\, W(t)\phi = ie^{+itH}\, Ve^{-itH_o}\, \phi \tag{2.2}$$

The technical domain conditions given below are chosen so that one

can justify (2.2).

THEOREM 2.2 (Cook's method). Suppose that $H\phi - H_o\phi \equiv V\phi$ for $\phi \in D(H) \cap D(H_o)$. Suppose moreover, there is a total set $\mathfrak{D} \subset D(H_o)$ so that $e^{-itH_o}\phi \in D(H)$ if $|t| \geq 1$ and that

$$\int_1^\infty \| V e^{\pm itH_o}\phi\| \, dt < \infty \tag{2.3}$$

for all $\phi \in \mathfrak{D}$. Then $\Omega^\pm(H,H_o)$ exist.

Proof. (2.2) holds by the domain hypothesis. Thus, by (2.3) we have that the right side of (2.1) goes to zero as $s,t \to \infty$ or as $s,t \to -\infty$. Proposition 2.1 completes the proof. Q.E.D.

Cook's method has been generalized to accommodate local singularities [17] and to accommodate form perturbations [31]. We want to describe how an estimate like (2.3) can be proven for $H_o = -\Delta$ and V's behaving like $r^{-1-\epsilon}$ at infinity. There seem to be three general techniques:

(a) (Kuroda [18]) Take $\mathfrak{D}$ to be the set of Gaussians $\phi_o = \exp(-a(x - x_o)^2)$ which are total. Using the explicit formula for $e^{-itH_o}\phi_o$, one easily proves (2.3) for any "reasonable" V.

(b) (Cook [6] used (2.5); the rest is folklore). Let ϕ be a nice smooth function with rapid falloff. Then certainly

$$\| e^{-itH_o}\phi\|_2 = \|\phi\|_2 \tag{2.4}$$

where

$$\|f\|_p = \left(\int |f(x)|^p dx\right)^{1/p}; \quad \|f\|_\infty = \text{ess.sup.}|f(x)|$$

Moreover, from the explicit integral kernel for e^{-itH_o}, i.e.

$$(e^{-itH_o}f)(x) = (4\pi it)^{-3/2}\int \exp(+(x - y)^2/2it)f(y)dy$$

one sees that

$$\| e^{-itH_o} \phi \|_\infty \leq t^{-3/2} \| \phi \|_1 \tag{2.5}$$

Hölder's inequality implies that

$$\| f \|_p \leq \| f \|_r^\theta \| f \|_q^{1-\theta} \quad ; \; p^{-1} = \theta r^{-1} + (1-\theta) q^{-1}$$

so, by (2.4) and (2.5)

$$\| e^{-itH_o} \phi \|_p \leq t^{-3(1/2-1/p)} \| \phi \|_1^{2/p} \| \phi \|_\infty^{1-2/p} \quad 2 \leq p \leq \infty \tag{2.6}$$

(Actually by using a more sophisticated tool, called complex interpolation, one can prove [2,7] that

$$\| e^{-itH_o} \phi \|_p \leq t^{-3(1/2 - 1/p)} \| \phi \|_{p'}$$

$$p' = (1 - p^{-1})^{-1} \; ; \; 2 \leq p \leq \infty) \tag{2.6'}$$

Using the general Hölder inequality

$$\| V\eta \|_p \leq \| V \|_r \| \eta \|_q \qquad p^{-1} = r^{-1} + q^{-1}$$

one sees that for nice enough ϕ ,

$$\| V e^{-itH_o} \phi \|_2 \leq C \, t^{-3/r} \| V \|_r \; ; \; r \geq 2 \tag{2.7}$$

As a result (2.3) holds for $H_o = -\Delta$ so long as $V \in L^2 + L^r$, $r < 3$. (Notice that $|r|^{-1-\varepsilon}$ is just barely in $L^2 + L^{3-\delta}$).

(c) (Advocated by Haag [3], used in [17] in weak form, raised to high art in [13]). To explain the idea, we explain it in one dimension. Let $(e^{-itH_o} u)(x) = u(x,t)$. Then, in terms of the Fourier transform

$$u(x,t) = (2\pi)^{-\frac{1}{2}} \int e^{ikx - ik^2 t} \hat{u}(k) \, dk \tag{2.8}$$

Now suppose that $\hat{u}$ is smooth and has support in some bounded set K.

Then, for $x/t \notin 2K = \{2k \mid k\epsilon K\}$ and $k\epsilon K$

$$\left(\frac{1}{ix - 2ikt}\frac{d}{dk}\right)^n e^{ikx - ik^2t} = e^{ikx - ik^2t}$$

Putting this in (2.8), and integrating by parts, one sees that

$$|u(x,t)| \leq C_n (1 + |x| + |t|)^{-n};\ x/t \notin (2 + \varepsilon) K$$

2K plays a special role here as the set of <u>classically allowed velocities</u> where the group velocity $\partial E(k)/\partial k$ is the relevant velocity. In three dimensions one has to break up $(\vec{x}, t, \vec{k})$ space into pieces since $(ix - 2ikt)^{-1} d/dk$ must be replaced by $[(ix - 2ikt)\cdot\rho]^{-1} d/d(k.\rho)$ for a suitable unit vector ρ, depending on where we are in $(\vec{x}, t, \vec{k})$ space. Being more explicit about the dependence of C_n on u, and using space translation invariance, one finds [13,32]:

$$|u(x,t)| \leq C_{n,\theta}(1 + |x - x_o| + |t|)^{-n} \| (1 + |x - x_o|)^n u\|_2 ;\ (x - x_o/t) \notin \theta \quad (2.9)$$

where $\frac{1}{2}\theta$ is any set containing the support of $\hat{u}$. To use this estimate to prove (2.3), we follow an idea of Enss [9]. Let $F(|x| \leq R)$ be the projection onto all functions supported in the set of x with $|x| \leq R$ etc. Let us suppose that V is bounded and

$$\int_1^\infty \| V\, F(|x| \geq R)\|\, dR < \infty \quad (2.10)$$

(this allows no local singularities but there are modifications which do; roughly speaking (2.10) says that V is $O(R^{-1-\varepsilon})$). Then

$$\| V e^{-itH_o} u\| \leq \| V F(|x| \geq \theta t) e^{-itH_o} u\| + \| V F(|x| \leq at)\, e^{-itH_o} u\|$$

$$\leq \| V F(|x| \geq at)\|\, \|u\| + \|V\|_\infty \| F(|x| \leq at) e^{itH_o} u\|_2 \quad (2.11)$$

The second term in (2.11) is L^1 in t by (2.9) so long as $\hat{u}$ is supported away from 0 and $a < \inf\{2k | k\varepsilon \text{ supp } \hat{u}\}$ and the first is in L^1 by (2.10) if $a > 0$. Thus (2.3) holds.

We close this section by answering a question that may have occurred to the reader: if the Gaussian wave packet argument ((a) above) works, why bother with the more sophisticated arguments (b), (c) above? Here is the answer:

(i) By working for general V's or wave functions, the alternate methods can be useful in situations which go beyond mere existence of $\Omega^{\pm}$; see, for example, § 6 where (2.9) plays an important role.

(ii) The Gaussian proof depends on having $H_o = -\Delta$. If H_o was a free Dirac Hamiltonian or if we want to describe impurity scattering in a solid, one of the other approaches would be more useful.

3 The Kato-Birman Theory (Trace Class Method)

In this section we want to describe a method initiated by T. Kato with further developments by M. Rosenblum, S. Kuroda, L. DeBranges, D. Pearson and most especially M.S. Birman and T. Kato. The simplest proof of the basic result is due to Pearson [24] and can be used as the basis of the whole theory [26].

Definition (a) For any bounded operator, A, on a Hilbert space, one defines its absolute value, $|A|$ to be $\sqrt{A^*A}$.

(b) For any A, $\sum_{n=1}^{\infty}(\phi_n, |A|\ \phi_n)$ is independent of the orthonomal basis $\{\phi_n\}$ chosen. The trace class, $\mathcal{C}_1$, is the set of A with the sum finite.

(b) $\mathcal{C}_p$ is the set of A with $|A|^p$ trace class. $\mathcal{C}_2$ is called the Hilbert-Schmidt operators.

We warn the reader that there are lots of subtleties in the theory (see [33] for a pedagogical overview); for example, $|A + B| \leq |A| + |B|$ (operator inequality) is false even for

2 x 2 matrices. Moreover, there are integral operators $(Af)(x) = \int K(x,y)\, f(y)dy$ with K continuous, and $\int |K(x,x)|dx < \infty$ but A not trace class. However, A is trace class if and only if A = BC with B,C Hilbert-Schmidt and an integral operator is Hilbert-Schmidt if and only if $\int |K(x,y)|^2\, dxdy < \infty$. Moreover, A trace class and B bounded implies AB trace class. The basic trace class scattering theorem depends on an abstract setup.

Definition Let A,B be self-adjoint operators and let $P_{ac}(A)$ be the projection onto the absolutely continuous subspace for A. Then, we say that $\Omega^{\pm}(B,A)$ exists if

$$\underset{t \to +\infty}{\text{s-lim}}\ e^{itB}\, e^{-itA}\, P_{ac}(A) \equiv \Omega^{\pm}(B,A)$$

exists and is complete if Ran $\Omega^{+}(B,A)$ = Ran $\Omega^{-}(B,A)$ = Ran $P_{ac}(B)$.

THEOREM 3.1 Suppose that either

(a) B-A is trace class

or (b) $(B + i)^{-1} - (A + i)^{-1}$ is trace class

or (c) A,B $\geq -c$ and $(A + c + 1)^{-1} - (B + c + 1)^{-1}$ is trace class.

Then $\Omega^{\pm}(B,A)$ exist and are complete.

We will not give a complete proof or various extensions (see [26]) but we will describe a few of the input ideas. One simple but basic idea is

THEOREM 3.2 Suppose that $\Omega^{\pm}(B,A)$ exist. Then they are complete if and only if $\Omega^{\pm}(A,B)$ exist.

This theorem means that existence under a condition symmetric in A,B implies completeness; see [7] for a multiparticle analog. Another important element is the use of a so-called invariance principle: i.e. that $\Omega^{\pm}(\phi(A), \phi(B)) = \Omega^{\pm}(A,B)$ for suitable ϕ's under suitable circumstances.

As for applications, we note:

THEOREM 3.3 Let $V \in L^1(R^3)$ and suppose that $H = -\Delta + V$ is such that $(H + i)^{-1}(H_o + i)$ is bounded. Then $(H + i)^{-1} - (H_o + i)^{-1}$

is trace class and, in particular, $\Omega^{\pm}(H,H_o)$ exist and are complete.

Proof Writing

$$(H + i)^{-1} - (H_o + i)^{-1}$$
$$= [(H + i)^{-1} (H_o + i)] [(H_o + i)^{-1}|V|^{\frac{1}{2}}] (\text{sgn } V)[|V|^{\frac{1}{2}}(H_o + i)^{-1}],$$

we see that it suffices to prove that $|V|^{\frac{1}{2}} (H_o + i)^{-1}$ is Hilbert-Schmidt. But this operator has an integral kernel $|V(x)|^{\frac{1}{2}} (4\pi|x - y|)^{-1} \exp(\alpha|x - y|)$, with $\text{Re}\alpha > 0$, $\alpha^2 = i$, which is clearly in $L^2(R^6)$ Q.E.D.

Roughly speaking, the condition $V \in L^1(R^3)$ requires that $V \sim |x|^{-3-\varepsilon}$ at infinity. If R^3 is replaced by R^ν, then one needs $|x|^{-\nu-\varepsilon}$. Since central potentials are one-dimensional, Kuroda [19] was able to use the trace class theory to prove existence and completeness of wave operators for central potentials obeying

$$\int_0^1 r|V(r)|dr + \int_1^\infty |V(r)|dr < \infty .$$

At first sight, trace class methods appear to be limited to two body problems but Combes [4] had the idea of applying them to N-body problems in the two-cluster regions; i.e. at energies below the lowest three body breakup. Simon [34] has extended this idea, and, in particular has proven:

THEOREM 3.4 Scattering of electrons off neutral atoms is complete below the energy necessary to ionize the atom.

At the present time, this is the only completeness result known for atomic scattering with more than one electron. We also note that Enss [10] has proven Theorem 3.4 with his methods.

4 Kato's Theory of Smooth Perturbations [16]

In this section, we want to say something about a remarkable theory of Kato [16] which has been extended in several ways by Lavine [21]. The basic definition is:

Definition Let A be self-adjoint. B is called A-smooth if and only if

$$\int_{-\infty}^{\infty} \| B\, e^{-itA}\, \phi\|^2\, dt \leq c\, \|\phi\|^2 \tag{4.1}$$

for all ϕ.

Example If $A = -\Delta$ on $L^2(R^3)$ and B is multiplication by a function in L^3, then B is A-smooth. Unfortunately, I know of no simple proof of this fact. The proof can be based on the estimate (2.6').

One use of this notion is seen in

THEOREM 4.1 Let $A = B + \sum_{i=1}^{n} C_i^* D_i$ and suppose that each D_i is A-smooth and each C_i is B-smooth. Then

$$\underset{t \to \pm\infty}{s\text{-}\lim}\ e^{itB}\, e^{-itA} \equiv U_{\pm} \tag{4.2}$$

exist, are unitary, and

$$U_{\pm}^{-1}\, B U_{\pm} = A \tag{4.3}$$

Proof We show existence of the limit. The fact that the limit is unitary follows from Theorem 3.2, and (4.3) from (1.11). Let ϕ, ψ be in our Hilbert space and write $W(t) = e^{itB}\, e^{-itA}$.

$$|(\phi, [W(t) - W(s)]\psi)| \leq \sum_{i=1}^{n} \int_s^t |(C_i\, e^{-iuB}\phi,\ D_i\, e^{-iuA}\, \psi)|\, du$$

$$\leq \Big(\sum_{i=1}^{n} \int_{-\infty}^{\infty} \| C_i\, e^{-iuB}\, \phi\|^2\, du\Big)^{\frac{1}{2}} \Big(\sum_{i=1}^{n} \int_s^t \| D_i\, e^{-iuA}\, \psi\|^2\, du\Big)^{\frac{1}{2}}$$

by the Schwartz inequality. Using (4.1) and the B-smoothness of C_i we see that

$$\| (W(t) - W(s)\psi\| \leq c(\sum_{i=1}^{n} \int_s^t \| D_i \, e^{-iuA} \, \psi\|^2 \, du)^{\frac{1}{2}}$$

Using the A-smoothness of D_i, we see that $\| (W(t) - W(s))\psi\| \to 0$ as $s,t \to \infty$. Q.E.D.

In thinking about applications of Theorem 4.1, it is useful to realize the strength of the conclusions. If $A = -\Delta$, B can have no bound states if Theorem 4.2 holds. One case where this is true is small coupling. The following was proven for N = 2 by Kato [26] and for general N by Iorio-O'Carroll [28]:

THEOREM 4.2 *For each* N, *there is a* Λ_N *so that, if* $\| V_{ij} \|_{3/2} < \Lambda_N$ $(1 \leq i < j \leq N)$, *then on* $L^2(R^{3N})$

$$H = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j} V_{ij} \, (r_i - r_j)$$

is unitarily equivalent to $H_o = -\Delta$ under the wave operators $\Omega^{\pm} \, (H, H_o)$.

The link between time-dependent and time-independent scattering theory is seen in the fact that the Fourier transform of $\chi_{(0,\infty)}(t) \, e^{-\varepsilon t} \, B \, e^{-iAt} \, \phi$ (with $\chi_{(0,\infty)}(t) = 0$, resp 1 if $t < 0$, resp $t \geq 0$) is $(2\pi)^{-\frac{1}{2}} \, (i)^{-1} B \, (A + \lambda - i\varepsilon)^{-1}$. By the Plancherel relation, (4.1) is equivalent to

$$\lim_{\varepsilon \downarrow 0} \int_{-\infty}^{\infty} [\| B(A + \lambda + i\varepsilon)^{-1} \, \phi\|^2 + \| B(A + \lambda - i\varepsilon)^{-1} \, \phi\|^2]$$

$$\leq 2\pi c \, \| \Phi\|^2$$

This shows a connection between scattering and boundary values of the resolvent. Since there are also connections between boundary values of the resolvent and the absence of singular spectrum (see Theorem 5.1 below), one has a relation between this problem and smoothness; in fact, one can prove:

THEOREM 4.3 *If* B *is* A-smooth *then* Ran B* *is in the absolutely*

continuous space for A.

A final criteria for smoothness we should mention is the following beautiful result of Kato [16]:

THEOREM 4.4 Let A,B be bounded self-adjoint operators and suppose that $i\,[A,B] \equiv D$ is non-negative. Then $C \equiv \sqrt{D}$ is A-smooth.

Proof. Note that

$$\int_s^t \| Ce^{-iuA}\phi\|^2\, du = \int_s^t i < e^{-iuA}\phi,\ [A,B]\ e^{-iuA}\phi > du$$

$$\equiv \int_s^t \frac{d}{du} < e^{-iuA}\phi,\ B\ e^{-iuA}\phi > du$$

$$\leq 2\ \|B\|\ \|\phi\|^2 \quad \text{Q.E.D.}$$

Lavine [21] noted that if $H = -\Delta + V$ where V is "repulsive" and if D is the generator of dilations, then formally $i[H,D] \geq 0$ so that modulo the technicalities of dealing with unbounded operators, smoothness techniques are available. Indeed, Lavine [21] has used Theorems 4.1 and 4.2 to prove absence of singular spectrum and completeness of wave operators for a large class of (even multiparticle) purely repulsive interactions.

5 The Weighted L^2-Space Method of Agmon and Kuroda [1,20]

Around 1970, Agmon [1] and Kuroda [20] developed what may well be the most powerful method for the study of the basic problems for two-body systems. The method is also useful in the study of multiparticle systems [5, 11, 12]. The method represents the culmination of two developments: the first concerns eigenfunction expansions obtained via Lippmann-Schwinger type equations. This development was initiated by Povzner, Ikebe and Faddeev and developed by a variety of others during the 60's. The second, which we describe below, concerns auxiliary Banach spaces and was developed most especially by Friedrichs, Rejto and Howland. In the late sixties Kuroda and Kato-Kuroda combined the methods and

the main issues concerned the best choice of auxiliary Banach space and a technical problem we mention below solved eventually by the "Agmon bootstrap".

The key to the solution of the completeness and singular spectrum problems by these methods is the control of boundary values of the resolvent. Singular spectrum is eliminated by (see [27]):

THEOREM 5.1 A sufficient condition for an operator, A, to have empty singular continuous spectrum is that there exists $p > 1$, a closed countable set $\mathcal{E}$, in R, and a dense set, X, in $\mathcal{H}$ so that for $[a,b] \subset R\backslash\mathcal{E}$ and $\phi \in X$.

$$\sup_{0 < \varepsilon < 1} \int_a^b |(\phi, (A - x - i\varepsilon)^{-1} \phi)|^p \, dx < \infty$$

In particular, if $(\phi,(A - \lambda)^{-1} \phi)$ is bounded as $\lambda \to R\backslash\mathcal{E}$, then A has no singular *continuous spectrum.*

As we saw in the last section, control of the resolvent also has something to do with completeness; this is most easily seen using Lavine's theory of local smoothness [21]. Now suppose that one tries to choose X to be a Banach space continuously embedded in $\mathcal{H}$. Then any $\phi \in \mathcal{H}$ defines a linear functional via $\chi \to (\phi,\chi)$ (Hilbert space inner product) so $\mathcal{H}$ is imbedded in X*. Of course as λ approaches the spectrum, the norm of $(A - \lambda)^{-1}$ as a map of $\mathcal{H}$ to $\mathcal{H}$ blows up but suppose that as a map of X to X* it does not. Then, so long as $\phi \in X$, $(\phi,(A - \lambda)^{-1} \phi)$ will be bounded as λ approaches the spectrum and we will have the necessary control on spectrum. One natural way of doing this is via a perturbation method. Suppose that $A = H_o + V$ and write

$$(H - \lambda)^{-1} = (H_o - \lambda)^{-1} (1 + V(H_o - \lambda)^{-1})^{-1} \tag{5.1}$$

The overall strategy is then the following:

(a) Pick X so that $(H_o - \lambda)^{-1}$ is bounded as a map of X to X*

(b) Pick V so that V maps X* to X and thus so that $V(H_o - \lambda)^{-1}$ is defined from the space X to <u>itself</u>.

(c) Show that $(1 + V(H_o - \lambda)^{-1})$ as a map from X to X is invertible as λ approaches points not in the point spectrum of H as a <u>map on</u> H.

(d) Prove that the point spectrum as a map on $\mathcal{H}$ lies in a closed countable set.

Notice that V must have smoothness or fall-off for (b) to hold and as X gets smaller, V must get nicer. Thus we want to choose X as large as possible and compatible with (a). For $H_o = -\Delta$, $\mathrm{Im}(H_o - x - i\varepsilon)^{-1}$ gives a $\pi\delta(p^2 - x)$ as $\varepsilon \to 0$, so X must consist of functions which are smooth enough to have meaning when multiplied by $\delta(p^2 - x)$. What is important is that $\int |\hat{\phi}(p)|^2\, \delta(p^2 - x)\, d^3p$ make sense for $\phi \in X$. A good choice is thus:

<u>Definition</u> $L^2_\delta = \{f \in L^2 \,|\, (1 + |x|^2)^{\delta/2} f \subset L^2\}$ with the obvious norm.

For $\delta > 0$, $L^2_\delta \subset L^2$ and with the L^2 duality, $(L^2_\delta)^* = L^2_{-\delta}$.

THEOREM 5.2 (<u>See [25]</u>). <u>Fix</u> $\delta > \frac{1}{2}$. <u>Then</u> $(-\Delta - \lambda)^{-1}$ <u>extends as a map of</u> L^2_δ <u>to</u> $L^2_{-\delta}$ <u>from</u> $\mathrm{Im}\,\lambda > 0$ <u>to</u> $\mathrm{Im}\,\lambda \geq 0$, $\lambda \neq 0$.

To get (b) to hold, it clearly suffices that

$$|V(x)| < C(1 + |x|)^{-1-\varepsilon} \tag{5.2}$$

and with a little more complication, one can accommodate local singularities.

Step (c) is somewhat trickier. First, one needs some kind of compactness which yields a Fredholm alternative so that non-invertibility can only occur if $V(H_o - \lambda)^{-1}\, \phi = -\phi$ has solutions in X. Then $\psi = (H_o - \lambda)^{-1}\, \phi$ obeys $H\psi = \lambda\psi$ but $\psi \in X^*$. If one can show $\psi \in L^2$, then (c) will be completed. This is accomplished by showing that if $\psi \in L^2_\alpha$, then the integral equations around imply that $\psi \in L^2_{\alpha + \frac{1}{2}\varepsilon}$ (the ε of (5.2)). Repeating this (the "Agmon

bootstrap") eventually gets $\psi \in L^2$. Problem (d) is also solved by the Agmon bootstrap and a compactness argument. The net result is (see [1, 20, 27]).

THEOREM 5.3 Suppose that, $(1 + |x|)^{1+\varepsilon} V \in L^2(R^3) + L^\infty(R^3)$. Then $H = -\Delta + V$ and $H_o = -\Delta$ obey

(a) $\Omega^{\pm}(H,H_o)$ exist and are complete

(b) H has empty singular continuous spectrum

6 Phase Space Analysis: The Method of Enss [9]

Within the last six months, a new method has been developed by V. Enss [9] with exciting potentialities. It has recovered Theorem 5.3 using entirely time-dependent methods and it can be extended to accommodate Coulomb potentials [10] and very likely multiparticle systems including atoms! [10]. The first step involves the fact that any state which is not bound is sure to leave the region of the potential at some time although it might return there. The following result is called the *RAGE theorem* after contributions of Ruelle [28], Amrein-Georgescu [2] and Enss; it is based on Wiener's theorem, (1.12):

THEOREM 6.1 Let F be any bounded operator with $F(H + i)^{-1}$ compact. Suppose that ϕ is orthogonal to $\mathcal{H}_{pp}$, the eigenvectors for H. Then

$$\frac{1}{2T} \int_{-T}^{T} \| F e^{-itH} \phi \|^2 \, dt \to 0 \tag{6.1}$$

Under the hypotheses of Theorem 5.3, one can show that $F(|x| \leq n)(H + i)^{-1}$ is compact, so using (6.1) we can choose $\tau_n > \tau_{n-1}$ so that

$$\| F(|x| \leq n) e^{-i\tau_n H} \phi \| \leq n^{-1} \tag{6.2}$$

Suppose that ϕ has energy spectral measure supported in some interval $[a,b]$, $0 < a < b < \infty$. Then, since $\phi_n \equiv e^{-i\tau_n H} \phi$ lives far from the scatterer one expects that the bulk of the momentum

in ϕ_n will lie in the region $a < k^2 < b$, since H and H_o look alike near infinity. This can be shown without too much trouble. Now one can make a decomposition $\phi_n = \phi_{n,in} + \phi_{n,out} + \phi_{n,w}$ where $\| \phi_{n,w} \| \to 0$ involves pieces which have momentum or x-space supports in the wrong region and $\phi_{n,out}$ (resp $\phi_{n,in}$) has momenta k so that k (resp - k) is not towards the scatterers. This requires a simultaneous decomposition in x and k space. Using (2.9) and the methods connected with the estimate (2.11), one shows that

$$\| (\Omega^- - 1)\, \phi_{n,out} \| \to 0 \quad ; \quad \| (\Omega^+ - 1)\, \phi_{n,in} \| \to 0$$

and thus

$$\| \phi_n - \Omega^- \phi_{n,out} - \Omega^+ \phi_{n,in} \| \to 0$$

It follows that any ϕ of the above type is automatically in Ran Ω^+ + Ran $\Omega^- \subset \mathcal{H}_{ac}$ so $\mathcal{H}_{sing} = \{0\}$. By a slightly more involved argument one shows that ϕ cannot lie in $(\text{Ran } \Omega^+)^\perp$. A density argument then yields the conclusions of Theorem 5.3.

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TOWARDS DISPERSION RELATIONS FOR ATOMIC SCATTERING

J.M. Combes

This lecture presents some recent applications of complex canonical transformation methods to the investigation of analyticity properties of two-body scattering amplitudes in N-particle systems interacting with Coulomb forces.

1 Introduction

Scattering theory for N-particle systems involving Coulomb forces presents a priori a set of fundamental problems which makes it appear as a very ambitious challenge of Mathematical Physics. In fact it has in addition to the difficulties inherent in many particle systems (such as existence, uniqueness and computation of scattering states) those linked with statistics and with the long range nature of the forces. However such systems also have very nice specific properties (e.g. homogeneity of the interactions, dilation analyticity) and one can expect in this explicit model to derive results on properties of scattering amplitudes not available for general N-particle systems by the methods actually known. The techniques presented here are based on complex canonical transformations; their relevance to analyticity properties of scattering amplitudes in the case of short range forces was stressed originally in [1] and [2]for the one particle problem and further developed in [3] and [4] for two body reactions involving ground state particles in non-relativistic multichannel systems. It appears however that this theory has to be supplemented by other techniques in order to provide complete results for the on-shell amplitudes. In particular local deformation techniques seem to be required for the analysis of excited atoms' amplitudes; unfortunately there does not exist yet a satisfactory operatorial treatment of such transformations for N-particle Hamiltonians, $N > 1$(the $N = 1$

case is treated in [5] [6] [7] [8]). On the other hand Agmon type estimates [9] for boundary values of Green's functions constitute another great lacunary part of the N-particle puzzle, in particular when long-range forces are involved; the asymptotic behaviour of these boundary values at large energies, well analysed for N = 1, is necessary to establish dispersion relations. Hopefully this field of mathematical analysis should make significant progress in the near future.

In the first part of this lecture we will give a brief description of the complex canonical transformation method; in Section 2 we will apply it to the analysis of approximate physical scattering amplitudes in the case of elastic two-body reactions involving ground-state composite particles. In the following sections we will present a program for a complete investigation of on-shell amplitudes in some typical problems involving Coulomb forces e.g. atom-atom, electron-atom and positron-atom scattering; we will show in particular how a partition technique can reduce the difficulties to those of a one-body problem, making available many of the results known in this case.

2 Complex Canonical Transformations

Consider an n-dimensional quantum system described by conjugate variables (X,P); $X, P \in R^n$. The corresponding operators on the Hilbert space $L^2(R^n)$ satisfy the canonical commutation relations:

$$(X_k, P_l) = i\,\delta_{kl} \quad (\hbar = 1) \tag{2.1}$$

It is easy to check that (2.1) is invariant under the real canonical transformations

$$X \to e^{\theta} X$$

$$P \to e^{-\theta} P \qquad , \theta \in R$$

and

$$X \to X$$

$$P \to P + \tau \qquad , \tau \in R^n$$

By Von-Neumann uniqueness theory these groups of canonical transformations are unitarily implementable. In the representation where the X_k's act as multiplication operators and

$$P_1 = - i \frac{\partial}{\partial X_1}$$

the corresponding unitary group $D(\theta)$ and $B(\tau)$ are given by

$$D(\theta) = \exp i \, (X.P + P.X)\theta \tag{2.2}$$

$$B(\tau) = \exp i \, \tau.X \tag{2.3}$$

(where . denotes the scalar product in R^n)

It is convenient to consider the semi-direct product L of these two groups of transformations which is called the Linear group [11] and is defined as the set of pairs (θ, τ), $\theta \in R$, $\tau \in R^n$, with the group law:

$$(\theta, \tau) \times (\theta', \tau') = (\theta + \theta', e^{-\theta'} \tau + \tau')$$

Its unitary representation on $L^2 (R^n)$ consistent with (2.2)(2.3) is given by:

$$(U(\theta, \tau) \phi) (X) = \exp(\frac{n\theta}{2}) \exp (- i \, X.\tau) \phi (e^{\theta}X) \tag{2.4}$$

Now let us investigate what happens if one allows complex values for θ and τ e.g. Im $\theta \in [- \frac{\Pi}{2} + \frac{\Pi}{2}]$ and $\tau \in R^n$. The canonical commutation relations(2.1) remain invariant; however since the new canonical variables are no more symmetric, unitary equivalence does not hold anymore. In fact the operators (2.2), (2.3) and (2.4) become unbounded. This lack of unitary equivalence is responsible for the radical change in the spectrum of the quantum Hamiltonian of the system under such a complex

canonical transformation of dynamical variables, although perturbation theory still allows us to have some control on the way this spectrum behaves under their effect. A nice fact is that this effect consists not only in disentangling some parts of the spectrum corresponding to a non-simple multiplicity (as for example in multichannel N-body systems) but also in "uncovering" some parts of the spectrum hidden on some unphysical Riemann sheets. (So they are not really part of the spectrum but however, their effect is felt e.g. through spectral concentration or, in a more familiar physical language, through resonances.)

The Transformed Hamiltonian

We assume that the system under consideration consists of N particles interacting via two-body potentials $V_{ij}, i,j = 1,\ldots,N$. The Hamiltonian has the form:

$$\frac{P_{CM}^2}{2M} + H = \sum_{i=1}^{N} \frac{P_i^2}{2m_i} + \sum_{i<j=1}^{N} V_{ij} \tag{2.5}$$

where $P_{CM} = \sum_{i=1}^{N} P_i$ and $M = \sum_{i=1}^{N} m_i$

Under reasonable assumptions on the V_{ij}'s (see e.g. [12]) H is self-adjoint on $L^2(R^{3N})$. We will assume here that the V_{ij}'s are both dilation and boost analytic. By this, we mean that the operators

$$V_{ij}(\theta) = D(\theta)\, V_{ij}\, D^{-1}(\theta) \qquad , \theta \in R$$

$$V_{ij}(\tau) = B(\tau) V_{ij}\, B^{-1}(\tau) \qquad , \tau \in R^n$$

are compact maps from the Sobolev space $W_2(R^3)$ (see [13]) to $L^2(R^3)$, having analytic extensions for complex values of θ and τ (i.e. analytic as compact operator valued functions). This holds in particular for Coulomb forces [3] [4]. Under those assumptions one has the following statement:

THEOREM 2.1 [10,11] Let H be as in (2.5) with dilation and boost analytic two-body potentials.

Let $\gamma = (\theta, \tau) \in L$ and

$$H(\gamma) = U(\gamma)\, H\, U^{-1}(\gamma)$$

(where $U(\gamma)$ is defined by (2.4)

Then for $Z \notin \sigma(H)$ there exists a complex neighbourhood of L in which $(H(\gamma) - Z)^{-1} = R(\gamma, Z)$ is analytic in each of the variables γ and Z. Furthermore:

i) The essential spectrum $\sigma_e(H(\gamma))$ is a union of parabolic domains $P_{\alpha,\theta}$ given by:

$$P_\alpha(\theta, I) = E_\alpha + e^{-2\theta}\{(P + \tau)^2_\alpha \quad , P \in R^{3N(\alpha)}\}$$

where

1) α is a channel of the system given by a partition $D(\alpha) = (C_1, C_2 \ldots C_{N(\alpha)})$ into $N(\alpha)$ clusters of the system and the specification of a given bound state energy $-E^{b(C)}$ for each cluster C in D;

Then $E_\alpha = \sum_{C \in D(\alpha)} E^{b(C)}$

2) $(P + \tau)^2_\alpha$ is the "kinetic energy" of the centers of mass of the clusters in $D(\alpha)$ after the complex boost τ has been performed.

Finally

ii) The point spectrum $\sigma_p(H(\gamma))$ is independent of γ as long as it is not absorbed by $\sigma_e(H(\gamma))$.

The proof of this theorem involves analytic perturbation theory [14]. One consequence of the analyticity of $R(\gamma, Z)$ is the consistency of the expectation values as functions of γ:

$$(\Phi, (H-Z)^{-1}\Psi) = (\Phi(\bar{\gamma}), R(\gamma,Z)\Psi(\gamma)) \qquad (2.6)$$

for all pairs of vectors Φ,Ψ locally analytic with respect to the linear group (i.e. such that $\Phi(\gamma) = U(\gamma)\Phi$, $\Phi \in L$, has an analytic continuation in a compex neighbourhood of L.)

Formula (2.6) will play a crucial role in the application of this theory to the investigation of analyticity properties of scattering amplitudes. Before doing it let us mention some other applications which are also directly relevant for this problem:

i) Resonance Calculations [12]

The above theorem shows that in the case where one takes $\tau = 0$ $\mathrm{Im}\theta \neq 0$, if there exists complex energy eigenvalues E of $H(\theta, 0)$ they necessarily stand in the half-plane $\mathrm{Im}E\mathrm{Im}\theta \geq 0$ and according to (2.6) they will give rise to poles on unphysical sheets of analytically continued expectation values $(\Phi,(H-Z)^{-1}\Psi)$ (Φ and Ψ belonging to the dense set of dilation analytic vectors).

Such poles should not be interpreted as resonances without some care; however in many physical situations and in particular for the Coulomb systems which will be described below, they also correspond to poles of the scattering amplitude and as such can be given an intrinsic physical interpretation.

The role of the statement ii) in the theorem is a stability criterion for variational calculations of $\sigma_p(H(\theta,0))$. The connection of this stability with an extended virial theorem has been discussed by E. Brandäs and P. Froelich [15].

ii) Spectral Properties of H and Scattering Theory

It is remarkable that under the rather weak decay properties imposed on the two-body forces, the spectra $\sigma_e(H(\theta,0))$ exhibit the typical structure that one would expect in a complete multichannel scattering system, in which the continuous part of H would be unitarily equivalent to a direct sum of Hamiltonians corresponding to all possible fragmentations of the N particle

system into non-interacting bound-states. Although this observation has not led to significant progress for the mathematical problem of asymptotic completeness (see however C. Van Winter Lecture) it certainly increases our conviction that, even for long-range forces, the continuous part of H consists of scattering states.

Let us mention as a by-product of part i) of Theorem 2.1 (in the case $\tau = 0$) and formula (2.6) that the continuous singular subspace of H is empty and that bound-states and resonances are discrete (isolated and finite multiplicity) accumulating at the most at threshold points E_α.

Finally a consequence of boost analyticity of $(H(\theta,\tau)-Z)^{-1}$ is the boost-analyticity of eigenvectors of H (even those embedded in the continuum) expressed for example by the fact that if $H\Phi = E\Phi$ then Φ is in the domain of the operator

$$e^{\theta(2M|E - E_\alpha| + \Gamma_\alpha)^{\frac{1}{2}} R}, \quad 0 < \theta < 1 ,$$

where R is the radius of gyration of the system and $E_\alpha + i\,\Gamma_\alpha$ is the closest real or complex threshold for E. This result can be extended to cover the case of systems having symmetries [16]. However it says less than parts i) and ii) of Theorem 2.1 together; the full content of these statements (see [11]) and subsequent L analyticity of bound-state wave-functions leads to more refined decay properties in some directions of configuration space, expressing the fact that some bound-states are "composite particles" whose constituents are in some sense themselves bound-states. In this respect such properties might be useful e.g. in variational calculations of molecular spectra. They will also be implicitly used later (Section 3) to investigate e.g. analyticity properties of exchange amplitudes.

3 Analyticity Properties of Approximate On-Shell Scattering Amplitudes

For the sake of generality we consider for the moment a general N-particle system with dilation and boost two-particle interactions; we will specify them later to be Coulomb interactions. A two-body reaction corresponds to a pair of asymptotic channels α defined by two-body cluster decompositions $D = (C_1^{\pm}, C_2^{\pm})$ and asymptotic bound state wave-functions $\Phi_{C_1^{\pm}}$, $\Phi_{C_2^{\pm}}$ describing the composite fragments built with particles in $C_1^{\pm}$, $C_2^{\pm}$ respectively. The off-shell scattering amplitude for this reaction is given by:

$$2\Pi^2 \, t\,(\underset{\sim}{k},\underset{\sim}{k}',Z) = < \Phi_{+,\underset{\sim}{k}'}, \tilde{V}_{D_-} \Phi_{-,\underset{\sim}{k}} >$$

$$+ < \tilde{V}_{D_+} \Phi_{+,\underset{\sim}{k}'}, (H-Z)^{-1} \tilde{V}_{D_-} \Phi_{-,\underset{\sim}{k}} > \qquad (3.1)$$

Asymptotic states $\Phi_{\pm,\underset{\sim}{k}}$ are defined as

$$\Phi_{\pm,\underset{\sim}{k}}(X) = (2\Pi)^{-3/2} \exp(i\underset{\sim}{k}.X_D)\, \Phi_{C_1^{\pm}}(X_{C_1^{\pm}})\, \Phi_{C_2^{\pm}}(X_{C_2^{\pm}})$$

Here X_D, X_C are Jacobi coordinates of X corresponding to the relative motion of clusters in D and particles in C respectively. We will concentrate mainly for simplicity on the special case of elastic forward scattering corresponding to $\alpha_+ = \alpha_-$ and $\underset{\sim}{k} = \underset{\sim}{k}'$. The approximate on-shell scattering amplitude corresponds to the choice:

$$Z = E_\alpha(k,\delta) = \frac{(k + i\delta)^2}{2M} + E_{C_1} + E_{C_2} + i\delta$$

where δ is an arbitrarily small positive number; the on-shell amplitude is obtained by letting $\delta \to 0$; M is a reduced mass for the two bound-states and E_{C_1}, E_{C_2} are negatives of their binding energies ($E^{b(C)} = 0$ if C consists of only one particle).

We will also investigate exchange amplitude for electron-atom scattering corresponding to $C_1^- = \{e_1\}$, C_2^- = ground-state atom(antisymmetric wave-function in the remaining (N-1) electron coordinates). The outgoing channel α_+ is obtained by exchanging electrons e_1 and e_2.

Since the first Born term on the right hand side of (3.1) is constant in the forward direction (elastic case), we only have to study

$$\Phi_\delta(k) = \langle \Psi_{+,\bar{\underset{\sim}{k}}} , (H - E_\alpha(k, \delta))^{-1} \Psi^c_{-,\underset{\sim}{k}} \rangle \tag{3.2}$$

For $k \in R$ we have $\bar{k}$ (complex conjugate of k) = k, but it is important to keep in mind the fact that we want to analytically continue in k and $< \Psi_{\bar{k}}$ is analytic in k if $\Psi_k >$ is where: $\Psi_{\pm,k} = V_{D_\pm} \Phi_{\pm,k}$ (we assume spherically symmetric bound-state wave-functions so that the forward amplitude only depends on $k = |\underset{\sim}{k}|$). For $k \in R^+$ formula (2.6) gives for any $\gamma \in L$:

$$\Phi_\delta(k) = \langle U(\gamma) \Psi_{+,\underset{\sim}{k}}, (H(\gamma) - E_\alpha(k,\delta))^{-1} U(\gamma)\Psi_{-,\underset{\sim}{k}} \rangle \tag{3.3}$$

The virtue of (3.3) is that for a suitable choice of $\gamma \in L$, usually dependent on $\underset{\sim}{k}$, one obtains new expressions for $\Phi_\delta(k)$ for which analyticity can be deduced entirely from Hilbert space considerations. As a first example let us consider elastic forward scattering of two ground-state composite particles such that $E_0 = E^{b(C_1)} + E^{b(C_2)}$ is the lowest threshold of H. We assume that two body interactions are such that Ψ_k is for $k \in R$ a square-integrable function; this happens for example as a consequence of screening when one considers scattering of a neutral atom by an electron or a positron or another atom [4]. We also need to assume dilation and boost analyticity of the bound state wave functions Φ_C which is a direct consequence of the theorem if two body interactions are.

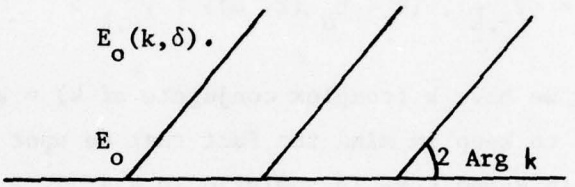
Example 1: Elastic forward amplitude

Choose $\gamma = \gamma_1(k) = (\log k, 0)$: then

$$U(\gamma)\Psi_k = \tilde{V}_D(k)\, \Phi_{C_1}(k) \otimes \Phi_{C_2}(k) \otimes e^{i\underset{\sim}{n}.X_D}$$

where $\underset{\sim}{n} = \underset{\sim}{k}/_k$, $\tilde{V}_D(k) = D(k)\, \tilde{V}_D\, D^{-1}(k)$, $\Phi_C(k) = D(k)\, \Phi_C$.

According to part (i) of Theorem 2.1 the essential spectrum of $H(\gamma_1(k))$ is (for complex k, Im k > 0) as indicated on the figure below:



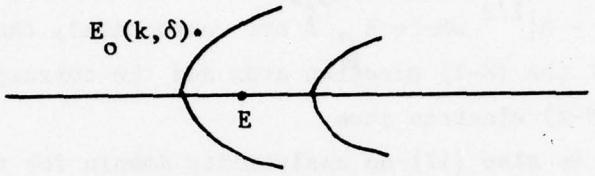
Since E_o is the lowest threshold of H the point $E_o(k,\delta)$ is never absorbed by the continuous spectrum of $H(\gamma_1(k))$ so that by the first part of the theorem $(H(\gamma_1(k)) - E_\alpha(k, \delta))^{-1}$ is at least for $\delta > 0$, an analytic operator valued function in $0 < \text{Arg } k < \Pi/2$; since this is also in general the natural analyticity domain for $U(\gamma_1(k))\, \Psi_k$, we conclude that $\Phi_\delta(k)$ can be analytically continued in $0 < \text{Arg } k < \Pi/2$. A similar method leads to analyticity in $\Pi/2 < \text{Arg } k \leq \Pi$. However the boundary Arg k = $\Pi/2$ cannot be reached with this choice of γ and we need to use a different transformation to include it in the analyticity domain. This will be done below but let us mention here that an extra virtue of $\gamma_1(k)$ is that it allows us also to perform analytic continuation on the first unphysical Riemann sheet corresponding to the branch point E_0; so poles of $(H(\theta) - Z)^{-1}$ on this unphysical sheet necessarily contain the singularities of the scattering amplitude. The problem of other sheets is more delicate.

Example 2: Elastic forward amplitude (continued)

Choose $\gamma = \gamma_2(\underset{\sim}{k}) = (0, \underset{\sim}{k})$; then

$$U(\gamma_2(\underset{\sim}{k}))\ \Psi_k = \tilde{V}_D\ \Phi_{C_1} \otimes \Phi_{C_2}$$

is k-independent. As to the essential spectrum of $H(\gamma_2(\underset{\sim}{k}))$ it consists of the interior of a set of parabolas as indicated below:



Since $E_\alpha(k, \delta)$ is never absorbed one has analyticity of $(H(\gamma_2(\underset{\sim}{k})) - E_o(k,\delta))^{-1}$ in Im k > 0 except at those values of $E_o(k,\delta)$ corresponding to eigenvalues of H.

Example 3: Exchange forward amplitude for e^- - neutral atom scattering [17]

One has

$$\Psi_{+,k} = (2\,\Pi)^{-3/2} \sum_{j \neq 1} \left(\frac{1}{|X_1 - X_j|} - \frac{1}{|X_1|}\right) \Phi_o(X_2, X_3, \ldots X_N)\ \exp(i\underset{\sim}{k}X_1)$$

$$\Psi_{-,k} = \sum_{j \neq 2} \left(\frac{1}{|X_2 - X_j|} - \frac{1}{|X_2|}\right) \Phi_0(X_1, X_3, \ldots X_N)\ \exp(i\underset{\sim}{k}X_2)$$

where Φ_0 is the ground state wave-function for a neutral atom with (N-1) electrons.

It is still possible to "dilate away" the k dependence of the plane-wave factors in $\Phi_{\pm,k}$ using the $\gamma_1(k)$ transformations; one obtains as in the elastic case analyticity in $0 < \text{Arg } k < \Pi/2$. However boost transformations $\gamma_2(\underset{\sim}{k})$ cannot be used anymore since now the boost must cancel simultaneously the two plane waves $\exp(-i\underset{\sim}{k}X_1)$ and $\exp(-i\underset{\sim}{k}X_2)$. So one takes the following boost $\tau = \tau(\underset{\sim}{k}) = (\underset{\sim}{k}, \underset{\sim}{k}, 0, \ldots 0)$ so that

$$B(\tau)\Phi_{+,k}(x_1,x_2,\ldots x_N) = (2\Pi)^{-3/2}\ \Phi_o(x_2,\ldots x_N)\ \exp(i\underset{\sim}{k}.x_2)$$

The above mentioned L-analyticity properties of bound-state wave-functions imply that $B(\tau)\ \Phi_{\pm,k}$ will be k-analytic in the domain $\text{Im}k < |E_o - \Lambda|^{1/2}$ where E_o, Λ are respectively the ground-state energy for the (N-1) electron atom and the corresponding ionized (N-2) electron atom.

This is also [17] an analyticity domain for the Born term of the amplitude and for $(H(0, \tau(k)) - E_0(k,\delta))^{-1}$; accordingly the exchange amplitude is meromorphic in the half-plane $\text{Im}k \geq 0$ but now with possible singularities (branch cut!) on $(i\ |E_o - \Lambda|^{1/2},\ i\ \infty)$. In the energy variable this would correspond to a left-hand cut $(-\infty,\ (E_o - \Lambda))$ as is expected in general for exchange amplitudes; notice that $|E_o - \Lambda|^{1/2}$ is precisely the rate of exponential fall off of the screened forces which electrons 1 and 2 are submitted to at large distances from the ionized atom.

Remark:

Scattering of excited particles

When E_α is not the lowest two-body threshold of the system the methods described in Section 3 do not work anymore since e.g. $E_\alpha\ (k,\ \delta)$ lies to the right of the first branch cut $E_o + e^{-2i\text{Arg}k}\ R^+$. In this case there is no transformation $\gamma(k)$ in the complex linear group such that $U(\gamma(k))\ \Psi_{\pm,k}$ and $(H(\gamma(k)) - E_\alpha(k,\ \delta))^{-1}$ are simultaneously analytic in some open set of the $\text{Im}k \geq 0$ half-plane. However for scattering of Coulomb particles the specific properties of atoms should allow the more refined technique of local distortions. This will be discussed in the next section.

4 The Partition Technique

The complex canonical transformation methods have given us

some insight into the type of results one can expect for the physical amplitudes. We describe now a complementary method which should allow us to deal with the remaining problems namely the $\delta = 0$ limit (physical amplitude), excited states and asymptotic behaviour. However the main advantage of this technique is to make available some of the results known for one-body problems and in this respect it is justified only by our lack of knowledge on mathematical properties of N-particle systems as mentioned in the introduction.

A more direct, although related, approach will be described in Dr. Singh's lecture using a suitable decoupling of singularities in the Weinberg-Van Winter equations.

Let $1 = P + Q$ be a partition of the identity operator, P being an orthogonal projection mapping. The following identity is standard and can be found e.g. in [18]:

$$(H-Z)^{-1} = (QHQ-Z)^{-1} + \{P+(QHQ-Z)^{-1}QHP\}G_P(Z)\ \{P+PHQ(QHQ-Z)^{-1}\}$$

where H is an arbitrary self-adjoint operator and

$$G_P(Z) = P(H-Z)^{-1}P$$

$$= P(PHP - PHQ(QHQ-Z)^{-1}QHP-Z)^{-1}P$$

In our case H will be the Hamiltonian (2.5) and P will be chosen in such a way that

1) PHP is essentially a Schrödinger matrix with one-body like diagonal elements involving only the canonical variables of the scattered electron.

2) QHQ has the same spectrum as H apart from the removal of those components corresponding to all channels having a lower threshold than the ones involved in the reaction. We also want this property to hold for the operators transformed under the complex linear group.

A consequence of this property is that for physical energies

$Z = E_\alpha(k)$ the resolvents $(Q(\gamma)H(\gamma)\ Q(\gamma)-E_\alpha(k))^{-1}$ will be analytic in $Imk > 0$ when γ is one of the k-dependent transformations defined in Section 3. However for $k\in R^+$ the point $E_\alpha(k)$ will be outside the essential spectrum of QHQ only up to the first threshold of QHQ that is, usually, under the three-body threshold of H; for larger energies this method is no more useful. So the result obtained in this way is that the physical amplitude exists pointwise in some limited range of energy and has analytic continuation in the upper half-plane. Finiteness of the total cross-sections at all energies remains an open problem although existence of wave operators guarantees that it holds in the average.

Choice of P

Let us consider a two-body reaction with asymptotic channels α_+ and α_- having threshold energies $E_{\alpha\pm} < \Lambda$ where Λ is the three-body threshold. Let E be such that $E_{\alpha\pm} < E < \Lambda$ and let P be the projection operator on $\mathcal{H}$

$$P\mathcal{H} = \{ \sum_{E_\alpha < E} \Phi_\alpha \otimes \xi_\alpha, \quad \xi_\alpha \in L^2(R^3)\} \tag{4.1}$$

where Φ_α is the bound-state part of the asymptotic wave function in channel α and ξ_α is the wave function describing the relative motion of the bound fragments. Then using standard results (see e.g. [19]) on the spectrum of Schrödinger Hamiltonians with relatively compact interactions one can show that $\sigma_e(QHQ) \subset (E, \infty)$; for the Hamiltonians $Q(\gamma)\ H(\gamma)\ Q(\gamma)$ transformed under elements of the complex linear group, the essential spectrum is exactly $\sigma_e(H(\gamma))$ but with those components (half-rays or parabolas) corresponding to channels α with $E_\alpha < E$ removed. If there are M channels of this type then $P\mathcal{H}$ is isomorphic to $(L^2(R^3))^M$ and PHP to an MxM matrix with operator valued elements which can be obtained in a straight forward way by computation. The diagonal

elements are one-body Schrodinger operators $h_\alpha = -\Delta + v_\alpha$; off-diagonal ones $v_{\alpha\beta}$ describing the coupling between channels; if $D(\alpha) \neq D(\beta)$ the coupling $v_{\alpha\beta}$ is a non-local operator having exponential fall-off properties as a consequence of the decay of the bound-state wave-functions Φ_α. If $D(\alpha) = D(\beta)$ then $v_{\alpha\beta}$ has at least as much decay properties as two-body interactions; in the case of Coulomb forces and neutral atoms, screening effects usually give an $0(1/r^2)$ decay and even exponential decay if α and β correspond to atomic states having the same parity. Such properties lead to finiteness of the number of bound-states for negatively charged atoms and one expects that they imply the equivalent finiteness of the total cross-section. We now make these arguments more explicit on some examples.

Example 1: Existence of the physical amplitude for positron (or electron) neutral atom scattering.

For positron-atom scattering for a ground state atom we take:

$$P\mathcal{H} = \{\Phi_o(x_2, \ldots x_N)\ \xi\ (x_1),\ \xi \in L^2\ (R^3)\ \} \tag{4.2}$$

where Φ_o is the atomic wave function and ξ is the positron wave function.

Then

$$PHP = (-\Delta_{x_1} + \tilde{V}(x_1) + E_o)\ P \tag{4.3}$$

where E_o is the negative binding energy and $\tilde{V}$ is the sum of positron electron interactions averaged over the electron density minus the positron-nucleus repulsion; $\tilde{V}$ has exponential fall-off and dilation analyticity so that we have a good one body problem; the energy dependent part in $G_p(Z)$, although non-local, has enough decay properties to be treated in perturbation theory.

If an electron is scattered instead of a positron one needs

to take (due to the identity of electrons).

$$P\mathcal{H} = \{ \sum_{\ell=1}^{N} \Phi_o (x_1 \ldots x_{\ell-1}, x_{\ell+1}, \ldots x_N) \xi^{(1)}(x_\ell) \} \qquad (4.4)$$

Diagonal elements of the N x N matrix associated with PHP will have the form (4.3); non-diagonal elements describe exchange forces and also have exponential decay.

Hence for these two problems the "complex" limiting absorption principle can be proved for Imk > 0 using Agmon-type estimates and the existence of the limits of $\Phi_\delta(k)$ as $\delta \to 0$ [9] follows for Imk > 0 or $E_\alpha(k) < E_1$ where E_1 is the energy of the first excited atomic state. We will see that the choice of P made in the next example can allow us in fact to prove existence of the physical amplitude up to the three-body threshold Λ and to analytically continue through the excited atom branch cuts.

Example 2: Excited atom scattering

Assume that the excited atoms involved in ingoing and outgoing channels have energies $E_{\alpha\pm}$ and consider an arbitrary E such that $E_{\alpha\pm} < E < \Lambda$. For positron scattering we take P of the form (4.1) where (Φ_α) is an orthogonal set of atomic wavefunctions with $E_\alpha < E$; for electron scattering one also has to sum as in (4.4) over all electron exchanges to take indistinguishability into account. The diagonal terms of PHP have the same structure as before and also the off-diagonal terms with $D(\alpha) \neq D(\beta)$.

If $D(\alpha) = D(\beta)$, i.e. if α and β differ only by the internal state of the atom, the off-diagonal element is a local potential with Fourier transform

$$\tilde{v}_{\alpha\beta}(P) = \int dP_1 \ldots dP_{j-1}\, dP_{j+1} \ldots dP_N\, \Phi(P_1, \ldots P_{j-1}, P_{j+1}, \ldots P_N)$$

$$\times \frac{1}{P^2} \sum_{i \neq j} \tilde{\Phi}_\beta(P_1, \ldots, P_i + P, \ldots, P_{j-1}, P_{j+1} \ldots P_N \qquad (4.5)$$

$$- \tilde{\Phi}_\beta(P_1, \ldots P_i, P_{j-1}, P_{j+1} \ldots P_N)$$

(This corresponds to the situation where electron j is scattered by the atom)

Since both Φ_β and Φ_α are boost analytic their Fourier transforms are analytic in a strip in every momentum variable P_i. If Φ_β and Φ_α have the same parity then P = 0 is a regular point and $\tilde{v}_{\alpha\beta}$ is analytic in a strip, which is equivalent by Paley-Wiener theorem to exponential fall-off of $v_{\alpha\beta}$. In general however P = 0 is a first order singularity and by expansion around P = 0 one obtains

$$\tilde{v}_{\alpha\beta}(\underset{\sim}{P}) = \frac{1}{P}\left(v^{(1)}_{\alpha\beta} + v^{(2)}_{\alpha\beta}\right)(\underset{\sim}{P})$$

where $v^{(1)}_{\alpha\beta}$ and $v^{(2)}_{\alpha\beta}$ are dilation analytic and analytic in a strip

$$|\mathrm{Im}P| < (\Lambda - E_\alpha)^{1/2} + (\Lambda - E_\beta)^{1/2}$$

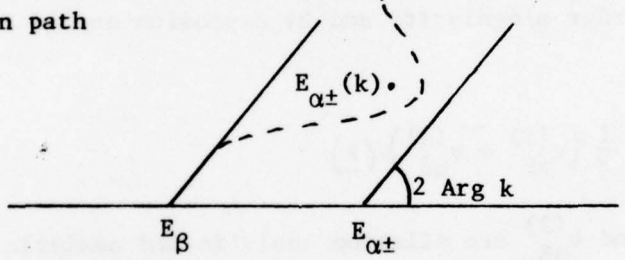
The singularity at P = 0 prevents exponential fall-off of $V_{\alpha\beta}$; the most one can expect is $O(|x|^{-1})$ $(x \to \infty)$ which is known to be the border line for existence of cross-sections. However here the specific form (4.5) will allow us to deal with this problem.

These analyticity properties also are those of the projected asymptotic states $P\Psi_{\pm,\underset{\sim}{k}}$; let us denote by $(\xi^{(\beta)}_k)_\beta$ the components of these states in the representation of $P\mathcal{H}$ as a Cartesian product of $L^2(R^3)$ spaces. The analyticity properties of the scattering amplitude in the elastic direct electron or positron

scattering will be essentially those of the matrix elements

$$< \xi_{\underset{\sim}{k}}^{-(\beta)}, (- \Delta + E_\beta - (E_{\alpha\pm} + k^2 + i0))^{-1} \xi_{\underset{\sim}{k}}^{(\beta)} > \qquad (4.6)$$

When k is complex, Imk > 0 two situations can occur; either $E_\beta > E_{\alpha\pm}$ in which case the branch cut $e^{2iArgk} R^+$ does not "absorb" $E_{\alpha\pm} - E_\beta + k^2$ when k varies in Imk > C and the complex dilation method of Section 2 works. Or $E_\beta \leq E_{\alpha\pm}$ then this method cannot be used without modification since in the complex rotation $\underset{\sim}{p} \to e^{2iArgk} \underset{\sim}{p}$ the branch cut $e^{2iArgk} R^+$ absorbs the point $E_\alpha(k) - E_\beta$ as soon as Imk > 0. However it is essential to notice that absorbtion occurs for a value of the momentum p which is a regular point of $\tilde{v}_{\alpha\beta}$ and $\xi_{\underset{\sim}{k}}^{(\beta)}$ whose only singularity is at $\underset{\sim}{q} = \underset{\sim}{k}$. Accordingly by a suitable local deformation of the p integration path



one should be able to avoid the non coincident singularity of the resolvent in (4.6). In fact each component $\xi^{(\beta)}$ inherits enough analyticity properties from (4.5) in order that such a deformation is possible [4]. It is then possible to prove for excited atoms the same analyticity properties of scattering amplitudes as in the ground-state case.

To conclude it is interesting to realize that the local deformation technique also allows us to perform analytic continuation of amplitudes on the unphysical sheets corresponding to the thresholds $(E_\beta - E_{\alpha\pm})^{\frac{1}{2}}$ where E_β is smaller than the three-body threshold Λ (and not only through the k = 0 threshold, this result being provided as we remarked above by dilation analyticity).

We hope that future mathematical progress will allow us to apply directly the local distortion method on the full N-particle Hamiltonian without having to use the partition technique as an intermediate step.

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SPECTRAL DENSITY AND SOJOURN TIMES

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The theory of smooth operators can be used to formulate mathematically and study the phenomenon of resonance for a single Hamiltonian operator, without reference to poles. In particular, upper and lower bounds for energy widths can be derived in certain cases.

1 What is a Resonance?

The phenomenon of resonance is very important physically, but it seems to resist mathematical formulation in a way that makes its physical meaning clear. The approach via analytic continuation of the resolvent has been very fruitful, but since any Hamiltonian can be given a resonance near any value in its spectrum by (im)proper choice of analytic continuation [1,8], its relevance ought to be demonstrated. In this paper we formulate the notion of resonance in terms of its physical effects. This leaves open the problem of showing the connection between analytic continuations of the resolvent and our criteria. We shall see, however, that some statements about resonance can be made in terms of these criteria alone.

When a Hamiltonian operator H for a quantum mechanical system has an eigenvalue λ, the physical consequences are

1) There is a state, represented by the eigenvector ψ, in which the energy is precisely λ,

2) If the system starts out in this state, it remains there forever.

When the system has a resonance near λ, this value is almost an eigenvalue in the sense that

1') There is a state whose energy distribution is highly concentrated near λ,

2') A system starting in this state remains there for a long time.

These two properties alone are not remarkable - in fact for any value λ in the spectrum a vector ψ can be found for which 1') and 2') hold, to any desired degree. Such behavior becomes noticeable when the state in question is also spatially localized, for

i) a given region of space can't support many states with concentrated energy; thus the peak stands out. (See §3)

ii) the system is spending a long time in a region which would normally be traversed more quickly.

There is another characteristic of eigenvalues which is important for computation.

3) The value of the function $\langle \phi, H\phi \rangle$ on the unit sphere $\{\|\phi\| = 1\}$ is stationary where ϕ is an eigenvector.

In Drachman's lecture at this conference it was pointed out that resonance has a similar characteristic:

3') The function $\langle \phi, H\phi \rangle$ varies slowly near ϕ.

This is a consequence of smallness of $(H - \lambda)\phi$, since if $\delta \perp \phi$

$$\langle \phi + \delta, H(\phi + \delta) \rangle = \langle \phi, H\phi \rangle + 2\mathrm{Re}\langle \delta, H - \lambda)\phi \rangle + \langle \delta, H\delta \rangle , \qquad (1.1)$$

so the first order term in δ is small if $(H - \lambda)\phi$ is small. Again, for any λ in the spectrum of H, $(H - \lambda)\phi$ can be made arbitrarily small for a suitable unit vector ϕ, but such functions ϕ, except in case of a genuine resonance, will be very spread out, and won't belong to the set of trial functions chosen for computation.

In section 2 we formulate the notions of energy width and lifetime using the language of smooth operators. In section 3 a quantity is defined which measures the local spectral density, and seems amenable to computation. In sections 4 and 5 we give estimates on the size of lifetimes and widths.

2 Energy Width and Sojourn Time

If A is a non-negative bounded operator on a Hilbert space $\mathcal{H}$, and H is a self-adjoint operator on $\mathcal{H}$, define the operator $\tau_H(A)$ by

$$\langle \phi, \tau_H(A)\phi \rangle = \int_{-\infty}^{\infty} \langle e^{-iHt}\phi, A\, e^{-iHt}\phi \rangle \, dt. \tag{2.1}$$

If A is a projection, the integrand is the probability of finding the solution of the Schrödinger equation in the subspace $\mathcal{R}(A)$ on which A projects, and $\langle \phi, \tau_H(A)\phi \rangle$ is the time spent by the solution in $\mathcal{R}(A)$.

Suppose T is a bounded operator on $\mathcal{H}$. Then if

$$\langle \phi, \tau_H(T^*T)\phi \rangle \leq C^2 \| \phi \|^2 \tag{2.2}$$

we say T is H-smooth, and the smallest such constant C is called $\|T\|_H$. (Our definition differs from that of Kato, who introduced these ideas [2], by a factor of 2π.)

If T is H-smooth, then for any $\phi \in \mathcal{H}$, $Te^{-itH}\phi$ is a square integrable function of t, which can be studied by considering $\langle \psi, Te^{-itH}\phi \rangle$ for various $\psi \in \mathcal{H}$. In particular, its Fourier transform satisfies

$$\begin{aligned} \langle \psi, \widehat{[Te^{-itH}\phi]}(\lambda) \rangle &= \langle \widehat{\psi, Te^{itH}\phi} \rangle \, (\lambda) \\ &= \lim_{\varepsilon \to 0} \frac{1}{\sqrt{2\pi}} \int_{\infty}^{\infty} e^{-\varepsilon t H} e^{-i\lambda t} \langle \psi, T\, e^{-itH}\phi \rangle \, dt \\ &= \lim_{\varepsilon \to 0} \frac{1}{\sqrt{2\pi}} \langle \psi, T[(H - \lambda - i\varepsilon)^{-1} - (H - \lambda + i\varepsilon)^{-1}]\phi \rangle \end{aligned} \tag{2.3}$$

Here the limit is taken in the sense of convergence in L^2. Take an orthonormal basis $\psi_1, \psi_2, \ldots$ for $\mathcal{H}$. Then

$$\| Te^{-itH}\phi \|^2 = \sum_{j=1}^{\infty} | \langle \psi_j, Te^{-itH}\phi \rangle |^2.$$

By integrating and using the Plancherel theorem for complex valued functions, we get

$$\int_{-\infty}^{\infty} \| Te^{-itH}\phi \|^2 dt = \frac{1}{2\pi} \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} \| T[(H-\lambda-i\varepsilon)^{-1} - (H-\lambda+i\varepsilon)^{-1}]\phi \|^2 d\lambda.$$

Now

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \| T[(H-\lambda-i\varepsilon)^{-1} - (H-\lambda+i\varepsilon)^{-1}]\phi \|^2 d\lambda$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} 4\varepsilon^2 \| T(H-\lambda-i\varepsilon)^{-1}(H-\lambda+i\varepsilon)^{-1}\phi \|^2 d\lambda$$

$$\leq \left\{ \sup_{\lambda \in \mathbb{R}} 2\varepsilon \| T(H-\lambda-i\varepsilon)^{-1} \|^2 \right\} \int_{-\infty}^{\infty} \frac{\varepsilon}{\pi} \| (H-\lambda+i\varepsilon)^{-1}\phi \|^2 d\lambda$$

$$= \sup_{\lambda \in \mathbb{R}} \{2\varepsilon \| T(H-\lambda-i\varepsilon)^{-1} \|^2\} \int_{-\infty}^{\infty} \frac{\varepsilon}{\pi} \| (H-\lambda-i\varepsilon)^{-1}\phi \|^2 d\lambda$$

$$= \sup_{\lambda \in \mathbb{R}} 2\varepsilon \| T(H-\lambda-i\varepsilon)^{-1} \|^2. \tag{2.4}$$

Thus $$\|T\|_H^2 \leq \lim_{\varepsilon \to 0} \sup_{\lambda \in \mathbb{R}} 2\varepsilon \| T(H-\lambda-i\varepsilon)^{-1} \|^2 \tag{2.5}$$

On the other hand, for any $\phi, \psi \in \mathcal{H}$

$$|\langle \psi, T(H-\lambda-i\varepsilon)^{-1}\phi \rangle|^2 = \left| \int_0^{\infty} e^{-\varepsilon t} e^{-i\lambda t} \langle \psi, e^{-iHt}\phi \rangle dt \right|^2$$

$$\leq \int_0^{\infty} e^{-2\varepsilon t} dt \int_{-\infty}^{\infty} \| Te^{-itH}\phi \|^2 dt \, \| \psi \|^2$$

$$\leq \frac{1}{2\varepsilon} \int_{-\infty}^{\infty} \| Te^{-itH}\phi \|^2 \| \psi \|^2 \tag{2.6}$$

So

$$2\varepsilon \| T(H-\lambda-i\varepsilon)^{-1} \|^2 \leq \|T\|_H^2 . \tag{2.7}$$

To summarize:

THEOREM 2.1. <u>For any</u> $\varepsilon > 0$ <u>and</u> $\lambda \in \mathbb{R}$,

$$2\varepsilon \|T(H-\lambda-i\varepsilon)^{-1}\|^2 \leq \|T\|_H^2 \leq \overline{\lim_{\varepsilon \to 0}} \sup_{\lambda \in \mathbb{R}} \|T(H-\lambda-i\varepsilon)^{-1}\|^2 .$$

Often one has estimates on $\|T(H-\lambda-i\varepsilon)^{-1}\|^2$ good only for a finite range of λ. In this case one says T is locally H-smooth. Such estimates imply bounds on lieftimes for states with energy in the specified range [4].

These results can be used to derive an energy-time uncertainty relation. In the P-Q relation, the uncertainties are usually represented by standard deviations. The result, though conceptually important, is technically not very useful. The standard deviation can be very large if the probability distribution has a long tail. For the Lorentzian

$$\delta_\varepsilon(\lambda-\lambda_0) = \frac{\varepsilon}{\pi} [(\lambda-\lambda_0)^2+\varepsilon^2]^{-1} \tag{2.8}$$

it is infinite! Instead, let us define the energy-width about λ_0 for a unit vector ϕ to be

$$\Delta E(\phi,\lambda_0) = \inf\{\varepsilon > 0: \pi\varepsilon \langle \phi, \delta_\varepsilon(H-\lambda_0)\phi \rangle \geq \tfrac{1}{2}\} \tag{2.9}$$

The quantity $\pi\varepsilon\langle \phi, \delta_\varepsilon(H-\lambda_0)\phi\rangle$ is an integral of the values of the energy distribution measure $d\langle\phi, E_\lambda\phi\rangle$ near λ_0. The smaller ΔE is, the more this measure is concentrated near λ_0. Note that $\pi\varepsilon\langle\phi, \delta_\varepsilon(H-\lambda_0)\phi\rangle = \varepsilon \|(H-\lambda_0-i\varepsilon)^{-1}\phi\|^2$.

Since $\pi\varepsilon\,\delta_\varepsilon(\lambda-\lambda_0)$ increases from 0 to 1 as ε runs from 0 to ∞ for $\lambda \neq \lambda_0$, and $\pi\varepsilon\,\delta_\varepsilon(0) = 1$ for all $\varepsilon > 0$, we have either

$$\Delta E > 0 \quad \text{and} \quad \pi\Delta E \langle \phi, \delta_{\Delta E}(H-\lambda_0)\phi\rangle = \tfrac{1}{2} \tag{2.10}$$

or $\Delta E = 0$, in which case λ_0 must be an eigenvalue.

PROPOSITION 2.2 <u>There exists</u> λ <u>in the spectrum of</u> H <u>such that</u> $|\lambda - \lambda_0| \leq \Delta E(\phi, \lambda_0)$.

<u>Proof</u>: Suppose there were no such λ. Then

$$\pi \Delta E \langle \phi, \delta_{\Delta E}(H-\lambda_0)\phi \rangle = \int \frac{(\Delta E)^2}{(\lambda-\lambda_0)^2 + \Delta E^2} \, d\langle \phi, E_\lambda \phi \rangle$$

$$< \frac{1}{2} \int d\langle \phi, E_\lambda \phi \rangle = \frac{1}{2}$$

which contradicts (2.10) #.

The time of sojourn in the state given by the unit vector ϕ, given initial value ψ, is $\langle \psi, \tau_H(|\phi\rangle\langle\phi|)\psi \rangle$. The relation between ΔE, standard deviation, and time of sojourn are given by

THEOREM 2.3 <u>If</u> ϕ <u>in a unit vector</u>,

$$\frac{1}{2} \langle \phi, \tau_H(|\phi\rangle\langle\phi|)\phi \rangle^{-1} \leq \Delta E(\phi, \lambda_0) \leq \| (H-\lambda_0)\phi \| \tag{2.11}$$

<u>Proof</u>: $1 = \langle \phi, \phi \rangle^2 = \left\{ \int \left[\frac{(\lambda-\lambda_0)^2 + \varepsilon^2}{\varepsilon} \right]^{\frac{1}{2}} \left[\frac{\varepsilon}{(\lambda-\lambda_0)^2 + \varepsilon^2} \right]^{\frac{1}{2}} d\langle \phi, E_\lambda \phi \rangle \right\}^2$

$$\leq \int \frac{(\lambda-\lambda_0)^2 + \varepsilon^2}{\varepsilon} \, d\langle \phi, E_\lambda \phi \rangle \int \frac{\varepsilon}{(\lambda-\lambda_0)^2 + \varepsilon^2} \, d\langle \phi, E_\lambda \phi \rangle$$

$$= \frac{\pi}{\varepsilon} \langle \phi, [(H-\lambda_0)^2 + \varepsilon^2]\phi \rangle \langle \phi \, \delta_\varepsilon(H-\lambda_0)\phi \rangle .$$

The expression $(\pi/\varepsilon)\langle \phi, [(H-\lambda_0)^2 + \varepsilon^2]\phi \rangle$ is minimized when $\varepsilon = \|(H-\lambda_0)\phi\|$, which gives, for all $\varepsilon > 0$,

$$1 \leq 2\pi \|(H-\lambda_0)\phi\| \langle \phi, \delta_\varepsilon(H-\lambda_0)\phi \rangle .$$

In particular, if $\Delta E > 0$, choosing $\varepsilon = \Delta E$ gives

$$1 \leq 2\pi \| (H-\lambda_0)\phi \| \langle \phi, \delta_{\Delta E}(H-\lambda_0)\phi \rangle$$

$$= \| (H-\lambda_0)\phi \| \frac{1}{\Delta E}$$

by (2.10), which is just the right hand inequality of (2.11). If $\Delta E = 0$, this inequality is trivial.

To prove the other inequality, note that for $\varepsilon > 0$ and $\lambda_0 \in \mathbb{R}$, (2.6) says

$$\langle \phi, \tau_H(|\phi\rangle\langle\phi|)\phi\rangle \geq 2\varepsilon |\langle \phi, (H-\lambda_0-i\varepsilon)^{-1}\phi\rangle|^2$$

$$\geq 2\varepsilon |\mathrm{Im}\langle \phi, (H-\lambda_0-i\varepsilon)^{-1}\phi\rangle|^2$$

$$= 2\varepsilon\pi^2 \langle \phi, \delta_\varepsilon(H-\lambda_0)\phi\rangle^2.$$

If $\Delta E > 0$, we may choose $\varepsilon = \Delta E$ and use (2.10) to get

$$\langle \phi, \tau_H(|\phi\rangle\langle\phi|)\phi\rangle \geq \frac{1}{2\Delta E} .$$

If $\Delta E = 0$, then ϕ has an eigenvector as a component, so $\langle \phi, \tau_H(|\phi\rangle\langle\phi|)\phi\rangle = \infty$. #

Thus to find a lower bound on the time of sojourn, it is enough to find an upper bound to $\Delta E(\phi,\lambda)$, i.e. to find a vector ϕ, value λ_0, and positive ε such that

$$\varepsilon \| (H-\lambda-i\varepsilon)^{-1}\phi \|^2 \geq 1/2\varepsilon \text{ ; then } \Delta E \leq \varepsilon.$$

3 Local Spectral Density

As emphasized in §1, a state may have narrow energy width (and therefore long lifetime) without being resonant. A long lifetime is remarkable only when the state is concentrated in a region which would normally be traversed in a short time. Narrow energy width is remarkable only when there are no other states of narrow width about nearby energies. The connection between these two conditions is that there is a limit to the number of states which can be concentrated in both energy and position.

It is not obvious how to formulate these notions precisely, but there is a quantity, the "local spectral density" $\rho(\lambda,x)$, which seems to be relevant. It is a measure on $\sigma(H)\times\mathbb{R}^n$ defined by

$$\int_{\sigma(H)}\int_{\mathbb{R}^n}|f(\lambda)\ g(x)|^2 d\rho(\lambda,x) = \mathrm{tr}(f(H)^*\ g(Q)^*\ g(Q)\ f(H))$$
$$= \| g(Q)f(H)\|_2^2 \qquad (3.1)$$

for suitable functions $f:\mathbb{R}\to\mathbb{C}$, and $g:\mathbb{R}^n\to\mathbb{C}$. (In (3.1) $\|\ldots\|_2$ denotes the Schmidt norm and $g(Q)$ is just the operator multiplication by g.)

Suppose that $n\le 3$ and let $H_0 = -\Delta$. Take $f(H) = \sqrt{\varepsilon}(H-\lambda_0-i\varepsilon)^{-1}$ and $g(Q) = \chi_B(Q)$, multiplication by the characteristic function of a bounded set $B\subset\mathbb{R}^n$.
Then

$$\varepsilon\|\chi_B(Q)(H-\lambda_0-i\varepsilon)^{-1}\|_2^2 = \varepsilon\|\chi_B(Q)(H_0-\lambda_0-i\varepsilon)^{-1}(1-V(H-\lambda_0-i\varepsilon)^{-1}\|_2^2$$
$$\le \varepsilon\|\chi_B(Q)(H_0-\lambda_0-i\varepsilon)^{-1}\|_2^2\ \|1-V(H-\lambda_0-i\varepsilon)^{-1}\|_2^2 \qquad (3.2)$$

The first factor on the right hand side can be calculated, since the operator is an explicitly known integral operator, and the second factor can be estimated by standard techniques if V is at all reasonable. The result is a bound on $\varepsilon\iint\chi_B(x)[(\lambda-\lambda_0)^2+\varepsilon^2]^{-1}$ $d\rho(\lambda,x)$ which is not too large for large ε, but blows up as $\varepsilon\to 0$. In other words we have a bound on an average of ρ over λ around λ_0, but not much idea of its fine structure.

On the other hand, if $\|\phi\| = 1$,

$$\varepsilon\|\chi_B(H-\lambda_0-i\varepsilon)^{-1}\phi\|^2 \le \varepsilon\|\chi_B(H-\lambda_0-i\varepsilon)^{-1}\|_2^2$$

$$= \varepsilon \int \chi_B(x) \left((\lambda-\lambda_0)^2 + \varepsilon^2\right)^{-1} d\rho(\lambda,x), \qquad (3.3)$$

which implies that $\int_{\mathbb{R}^n} \chi_B(x)\, d_x\rho(\lambda,x)$ is large near λ_0 if the left hand side is large. This may be expected to be the case with $\varepsilon \sim \Delta E(\phi,\lambda_0)$ if ϕ represents a state which is localized mostly in B and has small $\Delta E(\phi,\lambda_0)$.

The quantity $\rho(\lambda,x)$ can be approached in other ways. In fact for $n \leq 3$ it is given by $C\left[G(\lambda-i0;x,x) - G(\lambda+i0, x,x)\right]$, where G is the Green's function for H. This measure is a quantum analogue of the measure which assigns to the set $\Delta\lambda \times \Delta x$, the volume of the set of points in phase space with position in Δx and energy in $\Delta\lambda$. In fact it can be shown that if the dependence of ρ on Planck's constant is included, then ρ_h converges in a weak sense to this classical measure on $h \to 0$. The definition (3.1) of ρ in terms of a trace would seem to give a reasonable way to calculate ρ. (The theory of the spectral density will be developed elsewhere.)

4 Upper bounds on Lifetime

Upper bounds on τ_H are difficult in general. In fact such an estimate for $\tau_H(|V|)$ is a key to the problem of asymptotic completeness [3,6,7] in potential scattering. Since the arguments are complicated, let us consider the one dimensional Hamiltonian

$$H = -\frac{d^2}{dx^2} + V(x) \qquad (4.1)$$

operating in $L^2([0,\infty))$, with boundary condition $\phi(0) = 0$.

Suppose first that at energy λ, V has no barriers, i.e. $V(x) < \lambda$ for all $x \geq 0$. Assume V is differentiable and $\int_0^\infty |V'(x)|dx < \infty$. For any function g with $g(x) = 0$, a routine cal-

culation yields

$$\mathrm{Re}\langle g\frac{d}{dx}\,\phi,(H-\lambda)\phi\rangle = \frac{1}{2}\,\langle\phi',g'\phi'\rangle + \frac{1}{2}\,\langle\phi,[g(\lambda-V)]'\phi\rangle. \tag{4.2}$$

The right hand side can be made positive, in fact greater than an integrable function f^2, by solving

$$(\lambda-V)g' \geq V'g + f^2\ , \quad g' \geq 0. \tag{4.3}$$

Then subsituting $\phi = (H-\lambda-i\varepsilon)^{-1}\psi$ and using the Schwarz inequality on the left hand side of (4.2) gives

$$\varepsilon\|f(H-\lambda-i\varepsilon)^{-1}\psi\|^2 \leq \sup_{x\geq 0}|g(x)|\ \|\frac{d}{dx}(H-\lambda-i\varepsilon)^{-1}\psi\|\ \|\psi\|\,. \tag{4.4}$$

Since

$$\begin{aligned}\|\phi'\|^2 &= \langle\phi,(H-\lambda)\phi\rangle + \langle\phi,(\lambda-V)\phi\rangle \\ &\leq \langle\phi,(H-\lambda)\phi\rangle + (\lambda-V_0)\ \|\phi\|^2\end{aligned}$$

if $V(x) \geq V_0$ for all x, we have

$$\varepsilon\|f(H-\lambda-i\varepsilon)^{-1}\psi\|^2 \leq \sup_{x\geq 0}|g(x)|\ [\varepsilon+\lambda-V_0]^{\frac{1}{2}}\ \|\psi\|^2. \tag{4.5}$$

In other words, the operator of multiplication by f is H-smooth near λ.

A very important feature of quantum mechanics is that even if V does have a barrier, the particle spends only a finite (though possibly large) time inside the barrier. If V has a barrier, it can be split up as $V = V_1 + V_2$ where V_1 satisfies the above conditions and $V_2(x) \geq 0$, with $V_2(x) = 0$ *except for* $R_1 < x < R_2$. (The barrier is in the interval $[R_1,R_2]$).

One can solve

$$u''(x) = V_2(x)u(x),\ u(R_2) = 1,\ u'(R_2) = 0$$

on $[0,\infty)$. It is not hard to see that $u'(x) \leq 0$, and $u(x)=1$ for $x \geq R_2$. If the barrier is large, $u(0)$ may be extremely large.

Note that

$$\frac{1}{u} H \phi = \left[H - 2\frac{u'}{u} \frac{d}{dx} - \frac{u''}{u} \right] \frac{\phi}{u}$$

$$= \left[-\frac{d^2}{dx^2} - 2\frac{u'}{u} \frac{d}{dx} + V_1 \right] \frac{\phi}{u} \tag{4.6}$$

The right hand operator is a Hamiltonian without barriers, plus a first order differential operator. We can use the above argument, replacing the multiplier $g \frac{d}{dx}$ by $\frac{1}{u} g \frac{d}{dx} \frac{1}{u}$, because

$$\mathrm{Re} \left\langle \frac{1}{u} g \frac{d}{dx} \frac{\phi}{u} , (H-\lambda)\phi \right\rangle = \mathrm{Re} \left\langle g \frac{d}{dx} \frac{\phi}{u}, \left[-\frac{d^2}{dx^2} + V_1 - \lambda - 2\frac{u'}{u} \frac{d}{dx} \right] \frac{\phi}{u} \right\rangle$$

$$\geq \mathrm{Re} \left\langle g \frac{d}{dx} \frac{\phi}{u} , \left[-\frac{d^2}{dx^2} + V_1 - \lambda \right] \frac{\phi}{u} \right\rangle , \tag{4.7}$$

since $u'/u \leq 0$. By the argument for H without barriers,

$$\varepsilon \left\| \frac{1}{u} f (H - \lambda - i\varepsilon)^{-1} \psi \right\|^2 \leq \sup_{x \geq 0} g(x) \left\| \frac{d}{dx} \frac{1}{u} (H - \lambda - i\varepsilon)^{-1} \psi \right\| \left\| \frac{1}{u} \psi \right\| .$$

Now

$$\left\| \frac{d}{dx} \frac{\phi}{u} \right\|^2 = \left\| \frac{1}{u} \left(\frac{d}{dx} - \frac{u'}{u} \right) \phi \right\|^2 \leq \left\| \left[\frac{d}{dx} - \frac{u'}{u} \right] \phi \right\|^2$$

$$= \left\langle \phi, \left(-\frac{d^2}{dx^2} + \frac{u''}{u} \right) \phi \right\rangle$$

$$= \langle \phi, (H - V_1)\phi \rangle = \langle \phi, (H-\lambda)\phi \rangle - \langle \phi, (\lambda + V_1)\phi \rangle .$$

So it follows as before that

$$\varepsilon \left\| \frac{1}{u} f (H - \lambda - i\varepsilon)^{-1} \psi \right\|^2 \leq \sup_{x \geq 0} g(x) [\varepsilon + \lambda - V_0]^{\frac{1}{2}} \| \psi \|^2 . \tag{4.8}$$

The only difference is the factor $\frac{1}{u}$, which may be very small inside the barrier, thus making our estimate worse there.

Similar results are possible for $n (\geq 3)$ dimensional potential scattering with non-symmetric potentials [8], but there

are no such results for the $N(\geq 3)$ body problem.

5 Upper Bounds on Energy Width

To show the existence of resonance in our sense, we must find ϕ localized in space, with $\Delta E(\phi,\lambda)$ small compared to the spatial region where ϕ lives. We shall do this for a particle inside a potential barrier. Often resonance occurs upon perturbation of a Hamiltonian with an eigenvalue embedded in the continuum. Here there is no obvious choice of such an unperturbed operator. Instead we consider first a potential in which the barrier extends out to infinity so that the Hamiltonian has discrete spectrum at energies below the height of the barrier. Thus the perturbation is large, but only where the eigenfunctions (of the Hamiltonian with infinitely wide barrier) are small. In order to capitalize on this we need explicit estimates on decay of bound state eigenfunctions. Existing results on exponential decay do not rule out a bound state with most of its probability outside the potential well!

The following argument tells us that the particle is (probably) where it should be. (It can also be used to give a new proof of exponential decay in space.)

LEMMA 4.1 Let χ be a real bounded function on $\mathbb{R}^n$ with a bounded gradient. For all $\phi \in C_0^\infty(\mathbb{R}^n)$,

$$-\mathrm{Re}\langle \chi^2\phi, \Delta\phi\rangle = \|\nabla(\chi\phi)\|^2 - \|(\nabla\chi)\phi\|^2 \tag{5.1}$$

Proof.

$$\|\nabla(\chi\phi)\|^2 = \|(\nabla\chi)\phi + \chi\nabla\phi\|^2$$
$$= \|(\nabla\chi)\phi\|^2 + 2\mathrm{Re}\int \bar{\phi}\nabla\chi\cdot(\nabla\phi)\chi\, dx + \|\chi\nabla\phi\|^2.$$

Thus

$$\|\nabla(\chi\phi)\|^2 - \|(\nabla\chi)\phi\|^2 - \|\chi\nabla\phi\|^2 = \mathrm{Re}\int \bar{\phi}\nabla(\chi^2)\cdot\nabla\phi\, dx$$

$$= -\mathrm{Re} \int \phi\, \chi^2 \Delta\phi - \int \chi^2 |\nabla\phi|^2 \, dx. \quad \#$$

LEMMA 4.2 *If* χ *satisfies the conditions of Lemma 4.1, and* ϕ *is in the domain of* $-\Delta$, *then*

$$-\mathrm{Re}\langle \chi^2\phi, \Delta\phi\rangle + \| (\nabla\chi)\phi\|^2 \geq 0 \tag{5.2}$$

Proof. This ineqaulity follows from (5.1) for $\phi \in C_0^\infty(\mathbb{R}^n)$, and for ϕ in the domain of $-\Delta$ by taking limits in the inquality. #

By adding $\langle \phi, \chi^2(V-\lambda)\phi\rangle$ to both sides of (5.2) we obtain

PROPOSITION 5.3 *Let* V *be a measurable function such that* $H = -\Delta + V$ *is self-adjoint on the domain of* $-\Delta$. *Then if* $H\phi = \lambda\phi$, *and* χ *satisfies the conditions of Lemma 5.1*,

$$\langle \phi, (\chi^2(V-\lambda) - (\nabla\chi)^2)\phi\rangle \leq 0. \tag{5.3}$$

To get information about an eigenfunction ϕ, for a potential with a well, one makes a judicious choice of χ, so that χ is small in the well, grows as fast as possible in the classically forbidden region, consistent with the requirement that $\chi^2(V-\lambda) - (\nabla\chi)^2$ be positive. Thus χ becomes large far away from the well.

THEOREM 5.4 *Let* H *be as in Proposition 5.3, and suppose that there is a function* $v: [0,\infty) \to \mathbb{R}$ *such that* $V(x) \geq v(|x|)$, *with* $v(r) > \lambda$ *for* $r > R_1$. *Then if* $H\phi = \lambda\phi$,

$$\int_{|x|>R_2} (V(|x|) - \lambda)|\phi(x)|^2 dx \leq \exp\left[-2\int_{R_1}^{R_2} \sqrt{v(r)-\lambda}\, dr\right] \int_{|x|<R_1} (\lambda - V(x))|\phi(x)|^2 dx. \tag{5.4}$$

Proof. Take

$$\chi(r) = \begin{cases} 1 & r < R_1 \\ \exp \int_{R_1}^{r} \sqrt{v(s)-\lambda}\, ds & R_1 \leq r < R_2 \\ \exp \int_{R_1}^{R_2} \sqrt{v(s)-\lambda}\, ds & R_2 \leq r \end{cases}$$

Then $\nabla\chi(|x|) = 0$ except for $R_1 < |x| < R_2$, where

$$|\nabla\chi(x)|^2 = (v(|x|) - \lambda)\chi^2(x) \leq (V(x) - \lambda)\chi^2(x).$$

Then (5.4) follows from (5.3).#

One consequence of Theorem 5.4 is that eigenvalues are insensitive to the behavior of the potential far away in the classically forbidden region, because if $\tilde{V}(x) = V(x)$ for $|x| < R_2$, and $\tilde{H} = -\Delta + \tilde{V}$, then

$$\|(\tilde{H} - \lambda)\phi\|^2 = \|(\tilde{V} - V)\phi\|^2 = \int_{|x|>R_2} (\tilde{V} - V)^2 |\phi|^2$$

$$\leq \sup_{|x|>R_2} \frac{|\tilde{V}-V|^2}{V-\lambda} \exp\left\{-2\int_{R_1}^{R_2} \sqrt{v(r)-\lambda}\, dr\right\} \int_{|x|<R_1} [\lambda - V(x)]\, |\phi(x)|^2 dx,$$

which is small if the exponential factor is. But the spectrum of $\tilde{H}$ must contain a point whose distance from λ is no more than $\|(\tilde{H}-\lambda)\phi\|$. If $\tilde{V}$ is such that $\tilde{H}$ has only eigenvalues near λ, this point must be an eigenvalue.

Suppose, however, that $\tilde{V}$ has only a finite barrier. We claim that in this case $\tilde{H}$ has a resonance near λ.

THEOREM 5.5. Suppose that $H = -\Delta + V$ satisfies $H\phi = \lambda\phi$, and $V(x) \geq v(|x|)$, where $v(r) > \lambda$ for $r > R_1$ and for some $\alpha > \frac{1}{2}$, $v(r) > \lambda + \alpha^2/r^2$ for $r > R_2$. Suppose also that $\tilde{V}(x) = V(x)$ for $|x| < R_2$, but $\tilde{V}(x) < \lambda$ for large $|x|$ and $\tilde{H} = -\Delta + \tilde{V}$ is such that multiplication by

$$f(x) = \begin{cases} 0 & |x| < R_2 \\ \left|\frac{x}{R_2}\right|^{\alpha}, & |x| > R_2 \end{cases}$$

satisfies, for all $\varepsilon \neq 0$,

$$\varepsilon\| f(H-\lambda+i\varepsilon)^{-1}\|^2 = \varepsilon\| (H-\lambda-i\varepsilon)^{-1} f\|^2 \leq C^2. \tag{5.5}$$

Then the energy width for $\tilde{H}$ satisfies

$$\Delta E(\phi,\lambda) \leq 2C^2 \sup_{|x|>R_2} \frac{|V-\tilde{V}|^2}{V-\lambda-\frac{\alpha^2}{|x|^2}} \sup_{|x|<R_2} (\lambda-V) \exp\left(-2\int_{R_1}^{R_2} \sqrt{v(r)-\lambda}\, dr\right) \tag{5.6}$$

Proof.

$$\varepsilon\| (\tilde{H}-\lambda-i\varepsilon)^{-1}\phi\|^2 = \mathrm{Im}\langle \phi, (\tilde{H}-\lambda-i\varepsilon)^{-1}\phi\rangle$$

$$= \mathrm{Im}\langle \phi, \{(H-\lambda-i\varepsilon)^{-1} + (H-\lambda-i\varepsilon)^{-1}(V-\tilde{V})(H-\lambda-i\varepsilon)^{-1}$$

$$+ (H-\lambda-i\varepsilon)^{-1}(V-\tilde{V})(\tilde{H}-\lambda-i\varepsilon)^{-1}(V-\tilde{V})(H-\lambda-i\varepsilon)^{-1}\}\phi\rangle$$

$$= \mathrm{Im}\left\{\frac{\|\phi\|^2}{-i\varepsilon} + \frac{1}{(-i\varepsilon)^2}\langle \phi, (V-\tilde{V})\phi\rangle + \frac{1}{(-i\varepsilon)^2}\langle (V-\tilde{V})\phi, (H-\lambda-i\varepsilon)^{-1}\right.$$

$$\left.(V-\tilde{V})\phi\rangle\right\}.$$

The second term inside the brackets in the last expression is real. Therefore

$$\varepsilon\| (\tilde{H}-\lambda-i\varepsilon)^{-1}\phi\|^2 = \frac{1}{\varepsilon}\{\|\phi\|^2 - \frac{1}{\varepsilon}\langle (V-\tilde{V})\phi, (H-\lambda-i\varepsilon)^{-1}(V-\tilde{V})\phi\rangle\}$$

$$\geq \frac{1}{\varepsilon}\left\{\|\phi\|^2 - \frac{\varepsilon\| (H-\lambda-i\varepsilon)^{-1} f\|^2 \|f^{-1}(V-\tilde{V})\phi\|^2}{\varepsilon}\right\}$$

$$\geq \frac{1}{\varepsilon}\left\{\|\phi\|^2 - \frac{C^2}{\varepsilon}\|f^{-1}(V-\tilde{V})\phi\|^2\right\}.$$

The right hand side is maximized by choosing $\varepsilon = 2C^2\|f^{-1}(V-\tilde{V})\phi\|^2$, which gives $\|\varepsilon(H-\lambda-i\varepsilon)^{-1}\phi\|^2 \geq \frac{1}{2\varepsilon}$, so that

$$\Delta E(\phi,\lambda) \leq \varepsilon = 2C^2\|(V-\tilde{V})f^{-1}\phi\|^2. \tag{5.7}$$

To estimate the last factor, choose χ as in the proof of Theorem 5.4, except for $|x|>R_2$, where now

$$\chi(x) = \left(\frac{x}{R_2}\right)^{\alpha} \exp\left(\int_{R_1}^{R_2} \sqrt{v(r)-\lambda}\, dr\right).$$

Then by(5.3)

$$\int_{|x|>R_2} \left[V(x)-\lambda-\frac{\alpha^2}{|x|^2}\right]\left(\frac{x}{R_2}\right)^{2\alpha}|\phi(x)|^2dx \leq \exp\left(-2\int_{R_1}^{R_2}\sqrt{v(r)-\lambda}\,dr\right)$$

$$\times\int(\lambda-V)|\phi(x)|^2dx \leq \sup_{|x|<R_1}\left[\lambda-V_1\right]\exp -2\int_{R_1}^{R_2}\sqrt{v(r)-\lambda}\,dr\ . \qquad (5.8)$$
$$|x|<R_1$$

Then (5.6) follows from (5.7) and (5.8).#

It is important to note that the constant C^2 can be explicitly controlled. In (4.8), as long as f has support outside the barrier, C is of reasonable size, so that it does not compete with the exponential factor in (5.5). The same is true of the estimates for higher dimensions. [5].

A lower bound for $\varepsilon\|(\tilde{H}-\lambda-i\varepsilon)^{-1}\psi\|^2$ could be obtained much more easily by taking $\psi=(\tilde{H}-\lambda-i\varepsilon)\phi=(\tilde{V}-V-i\varepsilon)\phi$. This corresponds to bounding ΔE above by $\|(H-\lambda)\psi\|$. But the bound obtained is much worse, going as the square root of the exponential factor.

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STATIONARY TECHNIQUES FOR SCATTERING IN THE PRESENCE OF LONG-RANGE FORCES

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A review of three stationary formalisms for Coulomb scattering is given. Various integral formulations of the ionization S-matrix are examined.

1 Introduction

The difficulties associated with the usual short-range stationary scattering formalism when Coulomb potentials are present are well known [1]. For example the Lippmann-Schwinger equations for the two particle wave functions $\phi_{\pm}(\vec{x},\vec{p})$ given by

$$\phi_{\pm}(\vec{x},\vec{p}) = (2\pi)^{-3/2}\exp\,(i\,\vec{p}\cdot\vec{x}) - \frac{m}{2\pi}\int d\vec{y}\,\frac{\exp\,[\pm i\,p|\vec{x}-\vec{y}|]}{|\vec{x}-\vec{y}|}\,V(\vec{y})\,\phi_{\pm}(\vec{y},\vec{p}) \tag{1.1}$$

are not valid when V is a Coulomb-like potential since the integrals appearing in (1.1) do not exist (in the Lebesgue sense). Introducing space cut-offs or replacing (1.1) by the off-shell Lippmann-Schwinger equations leads to ill-defined limits and divergences in perturbation calculations.

In the first part of this talk we review three stationary formalisms for Coulomb scattering which circumvent the above difficulties. In section 2 a short account of the effective potential approach [7] for radial Coulomb scattering is given. The basic ideas of the "renormalized" space cut-off [3,9,13] and "renormalized" off-shell [15] approaches to Coulomb scattering are outlined in sections 3 and 4 respectively.

Much of our understanding of stationary scattering involving Coulomb potentials has been derived from Dollard's time-dependent theory of Coulomb scattering [2]. Using the time-dependent scattering theory as a basis for constructing time-independent scattering formalisms enables one to properly take into account

the asymptotic condition for Coulomb scattering. Furthermore since the time-dependent theory itself is valid for N-particle Coulomb scattering many of the stationary results are also valid in the N-particle scattering situation.

In the second part of this talk we review some recent work [17,18] on the ionization scattering amplitude which is based on the time-dependent scattering theory.

In section 5 we define "post", "prior", "plane wave-projected" and "Coulomb-projected" [5] versions of the half-shell T-matrix for ionization which formally reduce to the corresponding formulations of the ionization scattering amplitude on the energy-shell. The time-dependent scattering theory together with the relationship between the time-dependent and stationary scattering formalisms allow us to conclude that the post, plane wave-projected and Coulomb-projected half-shell T-matrices converge to zero in the energy shell limit while the prior version of the half-shell T-matrix converges to the physical S-matrix [17,18]. "Renormalized" versions of the post, plane wave-projected and Coulomb-projected half-shell T-matrix are defined and their convergence to the physical S-matrix is noted.

The results outlined in section 5 suggest that the various half-shell T-matrices which converge to zero in the energy-shell limit are discontinuous on the energy-shell. An explicit form of the discontinuity is conjectured in section 6.

In section 7 we discuss an approximate expression for the ionization S-matrix. The Born approximation for ionization is derived from this approximation under the assumption that the incident particle has a high relative energy compared to the ejected particle.

2 The Effective Potential Approach to Coulomb Scattering

From the well known asymptotic form of the Coulomb wave function it is clear that the breakdown of the Lippmann-Schwinger equations is related to their incompatibility with this asymptotic

form. This observation suggests two possible approaches to the formulation of an integral equation approach to Coulomb scattering: (1) Replace the free plane wave and free Green's functions in (1.1) by a "distorted free plane wave" and "distorted Green's functions". (2) "Undistort" the Coulomb wave functions appearing in (1.1). Both approaches have been used [4,7] to obtain generalized integral equations in the case of two particle radial Coulomb scattering. In this section we give a simplified account of the effective-potential approach, introduced in Ref. [7] for radial Coulomb scattering.

The radial wave function $u_\ell(x,p)$ satisfies the Schröedinger equation

$$\left(\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + p^2 - \frac{2me_1e_2}{x} - 2m\, V_s(x)\right) u_\ell(x,p) = 0 \tag{2.1}$$

and has the following asymptotic behaviour

$$u_\ell(x,p) \underset{x\to\infty}{\longrightarrow} \exp\left(i\delta_\ell(p)\right)\, \sin\left(px - \frac{\ell\pi}{2} - \gamma\, \ell n\, 2\, px + \delta_\ell(p)\right) \tag{2.2}$$

where $\gamma = \dfrac{me_1e_2}{p}$.

We introduce a function $h_\ell(x,p)$ defined as follows

$$h_\ell(x,p) = u_\ell\big(x + \phi(x,p),\ p\big) \tag{2.3}$$

where the function $\phi(x,p)$ is to be chosen so as to cancel $\gamma\, \ell n\, 2px$ appearing in (2.2). A natural choice for $\phi(x,p)$ is $\phi(x,p) = +\frac{\gamma}{p} g(x)\, \ell n\, 2px$ where $g(x)$ is an increasing C^3-function satisfying for some constants $R_2 > R_1 > 0$

$$g(x) = \begin{cases} 0 & \text{for } x \le R_1 \\ \\ 1 & \text{for } x \ge R_2 \end{cases}$$

For $\gamma>0$ with $p>0$ and for $\gamma<0$ with p sufficiently large the constants R_1 and R_2 can be chosen so that the effective potential (2.7) is nonsingular. The general case is treated in Ref. [7]. Using the fact that $u_\ell(x,p)$ satisfies the Schröedinger equation one obtains the following differential equation for $h_\ell(x,p)$ [7].

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + p^2 - q_{\ell,0}(x,p) - q_0(x,p) - q_1(x,p)\frac{d}{dx}\right] h_\ell(x,p)=0 \quad (2.4)$$

where

$$q_{\ell,0}(x,p) = V_s\Big[x + \phi(x,p)\Big] + \ell(\ell+1)\Big[\Big[x + \phi(x,p)\Big]^{-2} - x^{-2}\Big]$$

$$+ \{2\,\phi'(x,p) + [\phi'(x,p)]^2\}\left[\frac{\ell(\ell+1)}{[x + \phi(x,p)]^2} + V_s\,\big(x + \phi(x,p)\big)\right],$$

$$q_0(x,p)=-\{2\phi'(x,p) + [\phi'(x,p)]^2\}\left[p^2 - \frac{2me_1e_2}{x + \phi(x,p)}\right] + \frac{2me_1e_2}{x + \phi(x,p)} \quad (2.5)$$

and

$$q_1(x,p) = \phi''(x,p)\,[1 + \phi'(x,p)]^{-1}.$$

The transformation

$$h_\ell(x,p) = \psi_\ell(x,p)\big(1 + \phi'(x,p)\big)^{\frac{1}{2}}$$

leads to the following radial Schröedinger equation for $\psi_\ell(x,p)$

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + p^2 - q_\ell(x,p)\right] \psi_\ell(x,p) = 0 \quad (2.6)$$

where

$$q_\ell(x,p) = q_{\ell0}(x,p) + q_0(x,p) - \tfrac{1}{2}\, q_1'(x,p) + \tfrac{1}{4}[q_1(x,p)]^2. \quad (2.7)$$

Thus corresponding to the solution $u_\ell(x,p)$ of the radial Schröedinger equation with a Coulomb-like potential we have

associated a solution $\psi_\ell(x,p)$ of the radial Schröedinger equation (2.6) with an effective short-range potential $q_\ell(x,p)$ that is energy and angular momentum dependent. The function $\psi_\ell(x,p)$ has the following asymptotic behavior.

$$\psi_\ell(x,p) \underset{x\to\infty}{\longrightarrow} \exp\left(i\delta_\ell(p)\right) \sin\left(px - \frac{\ell\pi}{2} + \delta_\ell(p)\right) \tag{2.8}$$

The important point is that the phase shift in (2.8) is the same as the phase shift in (2.2), that is, $\frac{e_1e_2}{x} + V_s(x)$ and $q_\ell(x,p)$ are phase shift equivalent potentials.

The differential equation (2.6) together with (2.8) is equivalent to the integral equation

$$\psi_\ell(x,p) = j_\ell(x,p) + \int_0^{+\infty} dx'\ G_\ell^0(x,x')\ q_\ell(x',p)\ \psi_\ell(x',p) \tag{2.9}$$

The large x behavior of $\psi_\ell(x,p)$ leads to integral expressions for the partial wave scattering amplitudes [7].

The effective potential approach yields integral equations which can be solved by a convergent iterative procedure [7] and thus provides a method for the computation of the T-matrix for long-range scattering at a given value of the angular momentum.

3 Renormalized Space Cut-off Coulomb Scattering

Let $H(R)$ denote the space cut-off Hamiltonian defined by $H(R) = H_0 + g_R V_c + V_s$, $H_0 = -\frac{1}{2m}\nabla^2$ and $V_c(\vec{x}) = \frac{e_1e_2}{|\vec{x}|}$. For an appropriate class of cut-off functions $g_R(|\vec{x}|)$ [13] the cut-off dependent wave operators $W_\pm(R)$ defined by

$$W_\pm(R) = \underset{t\to\pm\infty}{\text{s-lim}} \exp(iH(R)t) \exp(-iH_0t)$$

exist and are related to the renormalized wave operators $\Omega_\pm$ via

[3,9,13]

$$\Omega_{\pm} = \underset{R\to\infty}{\text{s-lim}}\, W_{\pm}(R)\, \exp\left(\mp i\Lambda(R)\right) \tag{3.1}$$

where

$$\Lambda(R) = \frac{me_1e_2}{|\vec{p}|}\int_{t_0}^{+\infty} ds\, \frac{g_R\left(\frac{s|\vec{p}|}{m}\right)}{s} + \frac{me_1e_2}{|\vec{p}|}\log\left(\frac{2t_0|\vec{p}|^2}{m}\right) \tag{3.2}$$

for some constant $t_0 > 1$.

The operators $W_{\pm}(R)$ are related to the cut-off wave functions $\phi_{\pm}^R(\vec{x},\vec{p})$ via [6]

$$(W_{\pm}(R)\psi)(x) = \ell.i.m. \int \overrightarrow{dp}\, \phi_{\mp}^R(\vec{x},\vec{p})\, \hat{\psi}(\vec{p}). \tag{3.3}$$

Define "renormalized" cut-off wave functions $\tilde{\phi}_{\pm}^R(\vec{x},\vec{p})$ as follows: $\tilde{\phi}_{\pm}^R(\vec{x},\vec{p}) \equiv \phi_{\pm}^R(\vec{x},\vec{p})\exp\left(\pm i\Lambda(R)\right)$. The expansion (3.3) together with (3.1) yields the following relationship between the "renormalized" cut-off wave functions and the physical wave functions

$$\phi_{\pm}(\vec{x},\vec{p}) = \lim_{R\to\infty} \tilde{\phi}_{\pm}^R(\vec{x},\vec{p}) \tag{3.4}$$

where the above limit is to be understood in the sense of distributions [9,13].

The result (3.1) has been used to show the convergence of the "renormalized" cut-off T-matrix defined by

$$\left(\exp\left(2i\Lambda(R)\right) < \vec{p}|T(R)|\vec{p}'>\right)_{\frac{p^2}{2m} = \frac{p'^2}{2m}} \tag{3.5}$$

where

$$<\vec{p}|T(R)|\vec{p}'> = \int d\vec{x}\, (2\pi)^{-3/2} \exp(-i\vec{p}\cdot\vec{x})[(g_R V_c)(\vec{x}) + V_s(\vec{x})]\, \phi_+^R(\vec{x},\vec{p}')$$

to the physical Coulomb-like S-matrix [13].

The above "renormalized" cut-off formalism provides a general theoretical framework for understanding the removal of the space cut-off for the cut-off wave functions and T-matrix. The many calculations which have been performed with cut-off methods suggest that the removal of the cut-off is valid in a pointwise sense. We will come back to this point at the end of the next section.

Results analogous to those outlined in this section are valid in the case of general N-particle Coulomb scattering [9,13]. The anomalous phase factors appearing in the renormalized cut-off formalism can be calculated explicitly. Thus the renormalized cut-off formalism provides a basis for understanding the divergences appearing in the cut-off wave functions and T-matrices when the cut-off is removed.

4 Renormalized Off-shell Coulomb Scattering

The "renormalized" off-shell scattering formalism is based on the following representation for the renormalized wave operators [14]

$$\Omega_{\pm} = \underset{\varepsilon \to +0}{\text{s-lim}}\, W_{\pm\varepsilon}\, F_{\mp\varepsilon} \tag{4.1}$$

where

$$W_{\pm\varepsilon} = (\pm) \int_0^{\pm\infty} du\, \exp(\mp u)\, \exp(iH\, u/\varepsilon)\, \exp(-iH_0\, u/\varepsilon), \tag{4.2}$$

$$F_{\mp\varepsilon} = \Gamma(1 \pm i\gamma)^{-1} \exp\left[\pm i\gamma \log \frac{\varepsilon m}{2p^2}\right]$$

The representation (4.1) allows us to relate the off-shell wave functions $\phi_{\pm\varepsilon}(\vec{x},\vec{p})$ which satisfy the off-shell Lippmann-Schwinger equations

$$\phi_{\pm\varepsilon}(\vec{x},\vec{p}) = (2\pi)^{-3/2} \exp(i\, \vec{p}\cdot\vec{x}) - \frac{m}{2\pi} \int d\vec{y}\, \frac{\exp[ik|\vec{x}-\vec{y}|]}{|\vec{x}-\vec{y}|}\, V(\vec{y})\, \phi_{\pm\varepsilon}(\vec{y},\vec{p}) \tag{4.3}$$

where $k = \sqrt{p^2 \pm 2mi\varepsilon}$, to the physical Coulomb wave functions.

We first note that the operators $W_{\pm\varepsilon}$ can be expanded in terms of $\phi_{\pm\varepsilon}(\vec{x},\vec{p})$, i.e., [15]

$$(W_{\pm\varepsilon}\psi)(\vec{x}) = \int d\vec{p}\ \phi_{\mp\varepsilon}(\vec{x},\vec{p})\ \hat{\psi}\ (\vec{p}) \tag{4.4}$$

for each $\hat{\psi}\ \varepsilon C_0(R^3)$ and $\varepsilon > 0$.

Define "renormalized" off-shell wave functions $\tilde{\phi}_{\pm\varepsilon}(\vec{x},\vec{p})$ as follows: $\tilde{\phi}_{\pm\varepsilon}(\vec{x},\vec{p}) \equiv \phi_{\pm\varepsilon}(\vec{x},\vec{p})F_{\pm\varepsilon}$. The expansion (4.4) together with the presentation (4.1) yields.

$$\phi_{\pm}(\vec{x},\vec{p}) = \lim_{\varepsilon\to+0}\ \phi_{\pm\varepsilon}(\vec{x},\vec{p}) \tag{4.5}$$

where the above limit is taken in the sense of distributions. "Renormalized" half-shell and off-shell T-matrices can be defined and can be shown to have well defined energy-shell limits [15]. An alternative derivation of the relationship between the off-shell T-matrix and physical Coulomb S-matrix has been given by Veselova [12].

Similar results as outlined above for the two particle case have been shown for general N-particle Coulomb scattering [15]. Thus the renormalized off-shell formalism provides a framework for understanding the limit to physical energies of the off-shell wave functions and T-matrices.

The problem of applying the renormalized off-shell formalism to three particle Coulomb scattering is of particular interest since the various two particle off-shell quantities corresponding to the pure Coulomb potential are known in closed form. This, of course, is a prerequisite for the application of the Faddeev equations to scattering problems involving Coulomb potentials. It is hoped that the explicit knowledge of the divergences encountered when the solutions of the Faddeev equations are continued to physical energies (which is provided by the renormalized off-shell formalism) will eventually lead to computational results of use in atomic and molecular physics.

It is well known that the perturbation expansions associated with the Lippmann-Schwinger equations for the Coulomb cut-off and off-shell wave functions involve divergences in the limit $R \to \infty$ and $\varepsilon \to +0$ respectively. We expect that these divergences are related to the short-range asymptotic condition which is at the basis of the Lippmann-Schwinger equations. We do not expect divergences in the "renormalized" formalisms of section 3 and 4 since these formalisms are based on the correct asymptotic condition. The particular case of the renormalized off-shell Coulomb wave functions has been considered in detail in Ref. [16].

Let the formal iterative solutions to (4.3) with $V_s = 0$ be given by

$$\phi_{\pm\varepsilon}(\vec{x},\vec{p}) = \sum_{\ell=0}^{\infty} \gamma^{\ell}\, \phi_{\pm\varepsilon;\ell}(\vec{x},\vec{p}) \tag{4.6}$$

and the absolutely convergent expansions of $F_{\pm\varepsilon}$ be given by

$$F_{\pm\varepsilon} = \sum_{\ell=0}^{\infty} \gamma^{\ell}\, F_{\pm\varepsilon\ \ell}(|\vec{p}|) \tag{4.7}$$

The formal product of (4.6) and (4.7) is given by

$$\tilde{\phi}_{\pm\varepsilon}(\vec{x},\vec{p}) = \sum_{\ell=0}^{\infty} \gamma^{\ell}\, \Lambda_{\ell}(\vec{x},\vec{p};\ \pm\varepsilon) \tag{4.8}$$

where

$$\Lambda_{\ell}(x,p;\ \pm\varepsilon) = \sum_{n=0}^{\ell} F_{\pm\varepsilon;\ell-n}(|\vec{p}|)\ \phi_{\pm\varepsilon;n}(\vec{x},\vec{p}).$$

It has been shown [16] that the "renormalized" perturbation series (4.8) converges to the perturbation series for the pure Coulomb wave functions for $|\gamma| < 1$ in the limit $\varepsilon \to +0$. The resulting concept of a "renormalized" perturbation series has been extended to a general class of Coulomb-like potentials and to the renormalized half-shell T-matrix [16].

5 Half-shell T-matrices for Ionization

The problem of ionization is quite difficult from a theoretical viewpoint due to the long-range nature of the Coulomb potential. The usual integral formulations of the ionization scattering amplitude are not valid and thus the standard approximations for ionization, such as the Born and Coulomb-projected Born approximations [5], do not have an adequate justification. Generalized integral expressions have been developed [10], however the approximations based on these expressions have not led to good numerical results [11].

In order to discuss the various formulations of the ionization scattering amplitude we first outline some of our assumptions and introduce some notation.

In the sequel we consider the scattering of three distinct spinless charged particles with a Hamiltonian H given by

$$H = H_0 + V_{12} + V_1 + V_2$$

$$H_0 = -\frac{1}{2m_1}\nabla_1^2 - \frac{1}{2m_2}\nabla_2^2 ,$$

$$V_{12} = \frac{e_1 e_2}{|\vec{x}_1 - \vec{x}_2|} , \quad V_i = \frac{e_i e_N}{|\vec{x}_i|} , \quad i = 1,2$$

where m_i, $e_i = Z_i e$ and $\vec{x}_i$ represent respectively the mass, charge and position coordinate of particle i, $i = 1,2$, and e_N denotes the charge of the nucleus which is assumed to be infinitely heavy. We assume the initial channel α is made up of an uncharged fragment, consisting of particle 2 bound to the nucleus, and particle 1 free. We denote the bound state wave function by $\phi_\alpha(\vec{x}_2)$ and the corresponding bound state energy by E_α. The final channel consists of three free charged particles.

We denote the two particle Coulomb wave function corresponding to incoming boundary conditions by $\psi_-(\vec{x}_i,\vec{p}_i)$, $i = 1,2$, where $\vec{p}_i$ is the momentum of particle i, $i = 1,2$. The incoming wave

function corresponding to the free channel and outgoing wave function corresponding to the channel α are denoted respectively by $\phi_-(\vec{x}_1,\vec{x}_2;\ \vec{p}_1,\vec{p}_2)$ and $\phi^{(\alpha)}(\vec{x}_1,\vec{x}_2;\ \vec{p}_1)$. The initial energy of the system is given by $E_i = \frac{|\vec{p}_1|^2}{2m_1} + E_\alpha$ and the final energy of the system is given by $E_f = \frac{|\vec{p}_1|^2}{2m_1} + \frac{|\vec{p}_2|^2}{2m_2}$.

The various half-shell T-matrices for ionization which are considered in this section are defined in Table I via the following formal expression

$$\langle \vec{p}_1,\vec{p}_2|T|\vec{p}_1'\rangle = \lim_{R\to\infty} \pi^{-1}\int d\vec{x}_1 d\vec{x}_2\ \overline{\phi_f(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)} \times \exp\left(-\frac{1}{R}\,(|\vec{x}_1|+|\vec{x}_2|)\right) V(\vec{x}_1,\vec{x}_2)\ \phi_i(\vec{x}_1,\vec{x}_2;\vec{p}_1') \tag{5.1}$$

where the limit $R \to \infty$ is to be taken in the sense of distributions [17,18].

It is possible to relate the half-shell T-matrices defined by Table 1 to various expressions appearing in the time-dependent theory of scattering. The time-dependent theory can then be used to examine the behavior of these half-shell T-matrices in the energy-shell limit. This type of argument has been used [17,18] to show that the post, plane wave-projected and Coulomb-projected formulations of the half-shell T-matrix converge to zero in the energy-shell limit, i.e.,

$$\lim_{\varepsilon\to+0} \int d\vec{p}_1 d\vec{p}_2 d\vec{p}_1'\ \hat{f}(\vec{p}_1,\vec{p}_2)\ \hat{g}(\vec{p}_1')\ \ T(\vec{p}_1,\vec{p}_2;\vec{p}_1')\ \frac{\varepsilon}{(E_f-E_i)^2+\varepsilon^2} = 0 \tag{5.2}$$

where $T(\vec{p}_1,\vec{p}_2;\vec{p}_1')$ represents either T_{PT}, T_{PP} or T_{CP} and $\hat{g} \in C_0^\infty(R^3\backslash\{0\})$, $\hat{f} \in \mathcal{D}$, $\mathcal{D} = \{\hat{h}(\vec{p}_1,\vec{p}_2) \in C_0^\infty(R^6)\,|\,\hat{h}(\vec{p}_1,\vec{p}_2) = 0$ in a neighborhood of each of the sets $\vec{p}_1 = 0$, $\vec{p}_2 = 0$ and $m_1\vec{p}_2 = m_2\vec{p}_1\}$.

TABLE I. Definition of the post, prior, plane wave-projected and Coulomb-projected half-shell T-matrices.

T-matrix	denoted	$\phi_i(\vec{x}_1,\vec{x}_2;\vec{p}_1')$	$\phi_f(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)$	$V(\vec{x}_1,\vec{x}_2)$
post	T_{PT}	$\psi^{(\alpha)}(\vec{x}_1,\vec{x}_2;\vec{p}_1')$	$(2\pi)^{-3}\exp(i\vec{p}_1\cdot\vec{x}_1+i\vec{p}_2\cdot\vec{x}_2)$	$V_{12}+V_1+V_2$
prior	T_{PR}	$(2\pi)^{-3/2}\exp(i\vec{p}_1'\cdot\vec{x}_1)\phi_\alpha(\vec{x}_2)$	$\psi_-(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)$	$V_{12}+V_1$
plane wave-projected	T_{PP}	$\psi^{(\alpha)}(\vec{x}_1,\vec{x}_2;\vec{p}_1')$	$(2\pi)^{-3/2}\exp(i\vec{p}_1\cdot\vec{x}_1)\psi_-(\vec{x}_2,\vec{p}_2)$	$V_{12}+V_1$
Coulomb-projected	T_{CP}	$\psi^{(\alpha)}(\vec{x}_1,\vec{x}_2;\vec{p}_1')$	$\psi_-(\vec{x}_1,\vec{p}_1)\psi_-(\vec{x}_2,\vec{p}_2)$	V_{12}

The breakdown of the energy-shell limit of T_{PT}, T_{PP} and T_{CP} is due to their definition which does not correctly take into account the asymptotic condition for Coulomb scattering.

In contrast to T_{PT}, T_{PP} and T_{CP} the prior form of the half-shell T-matrix converges in the energy-shell limit to the physical ionization S-matrix denoted $\langle \vec{p}_1, \vec{p}_2 | S | \vec{p}_1' \rangle_{E_f=E_i}$. This is in part due to the "screening" effect of the potential appearing in T_{PR}. However, Coulomb difficulties are still present since the evaluation of the ionization S-matrix via the prior form of the half-shell T-matrix requires a knowledge of $\psi_-(\vec{x}_1, \vec{x}_2; \vec{p}_1, \vec{p}_2)$. We consider this problem in section 7.

Although the post, plane wave-projected and Coulomb-projected half-shell T-matrices do not have physical energy-shell limits it is possible to define "renormalized" half-shell T-matrices which converge to the ionization S-matrix [15,18]. Let $\Lambda_{PT}(\varepsilon)$, $\Lambda_{PP}(\varepsilon)$ and $\Lambda_{CP}(\varepsilon)$ be given by

$$\Lambda_{PT}(\varepsilon) = \Gamma(1-ih)^{-1} \exp\left\{ -ih_{12} \log\left[\frac{\varepsilon m_1 m_2 (m_1+m_2)}{2|m_2\vec{p}_1 - m_1\vec{p}_2|^2}\right] - ih_1 \log\left[\frac{\varepsilon m_1}{2|\vec{p}_1|^2}\right] - ih_2 \log\left[\frac{\varepsilon m_2}{2|\vec{p}_2|^2}\right]\right\},$$

$$\Lambda_{PP}(\varepsilon) = \Gamma(1-i\{h_{12}+h_1\})^{-1} \exp\left\{ -ih_{12} \log\left[\frac{\varepsilon m_1 m_2 (m_1+m_2)}{2|m_2\vec{p}_1 - m_1\vec{p}_2|^2}\right] - ih_1 \log\left[\frac{\varepsilon m_1}{2|\vec{p}_1|^2}\right]\right\} \tag{5.3}$$

$$\Lambda_{CP}(\varepsilon) = \Lambda_{PT}(\varepsilon)\Big|_{e_N=0}$$

where $h = h_{12} + h_1 + h_2$, $h_{12} = \dfrac{m_1 m_2 e_1 e_2}{|m_2\vec{p}_1 - m_1\vec{p}_2|}$, $h_i = \dfrac{m_i e_i e_N}{|\vec{p}_i|}$, $i = 1,2$.

The "renormalized" post, plane wave-projected and Coulomb-projected half-shell T-matrices are defined respectively by $T_{RPT} \equiv \Lambda_{PT}(\varepsilon)T_{PT}$, $T_{RPP} \equiv \Lambda_{PP}(\varepsilon)T_{PP}$ and $T_{RCP} \equiv \Lambda_{CP}(\varepsilon)T_{CP}$. These renormalized half-shell T-matrices converge to the physical S-matrix in the following sense [15,18]

$$\lim_{\varepsilon \to +0} \int d\vec{p}_1 d\vec{p}_2 d\vec{p}_1' \, \overline{\hat{f}(\vec{p}_1,\vec{p}_2)} \, \hat{g}(\vec{p}_1') \, T_\varepsilon(\vec{p}_1,\vec{p}_2;\vec{p}_1') \, \frac{\varepsilon}{(E_f-E_i)^2+\varepsilon^2}$$

$$= \int_{E_f=E_i} d\vec{p}_1 d\vec{p}_2 d\vec{p}_1' \, \overline{\hat{f}(\vec{p}_1,\vec{p}_2)} \, \hat{g}(\vec{p}_1') \, \langle \vec{p}_1,\vec{p}_2|S|\vec{p}_1' \rangle_{E_f=E_i}$$

where $T_\varepsilon(\vec{p}_1,\vec{p}_2;\vec{p}_1')$ represents either T_{RPT}, T_{RPP} or T_{RCP} and

$\hat{g} \in C_0^\infty(R^3\backslash\{0\})$, $\hat{f} \in \mathcal{D}$.

6 Singularity Structure of the Half-shell T-matrix

The results outlined in section 5 are compatible with the following behavior of the post, plane wave-projected and Coulomb-projected half-shell T-matrices as $E_f - E_i \to 0$

$$T_{PT} = \tilde{\Lambda}_{PT} T^1_{PT} + T^2_{PT} \tag{6.1}$$

$$T_{PP} = \tilde{\Lambda}_{PP} T^1_{PP} + T^2_{PP} \tag{6.2}$$

and

$$T_{CP} = \tilde{\Lambda}_{CP} T^1_{CP} + T^2_{CP} \tag{6.3}$$

where

$$\tilde{\Lambda}_{PT} = \Gamma(1-ih)|E_f-E_i|^{ih} \exp\left\{ih_{12} \log\left[\frac{m_1 m_2 (m_1+m_2)}{2|m_2\vec{p}_1 - m_1\vec{p}_2|^2}\right]\right.$$

$$+ ih_1 \log\left[\frac{m_1}{2|\vec{p}_1|^2}\right] + ih_2 \log\left[\frac{m_2}{2|\vec{p}_2|^2}\right]\Bigg\} \times \begin{cases} \exp\left(-\frac{\pi h}{2}\right) & E_f > E_i \\ \exp\left(\frac{\pi h}{2}\right) & E_f < E_i \end{cases}$$

$$\tilde{\Lambda}_{PP} = \Gamma(1-i\{h_{12}+h_1\})|E_f-E_i|^{i\{h_{12}+h_1\}} \exp\Bigg\{ih_{12} \log\left[\frac{m_1 m_2 (m_1+m_2)}{2|m_2\vec{p}_1 - m_1\vec{p}_2|^2}\right] \tag{6.4}$$

$$+ ih_1 \log\left[\frac{m_1}{2|\vec{p}_1|^2}\right]\Bigg\} \times \begin{cases} \exp\left(-\frac{\pi}{2}\{h_{12}+h_1\}\right) & E_f > E_i \\ \exp\left(\frac{\pi}{2}\{h_{12}+h_1\}\right) & E_f < E_i \end{cases}$$

$$\tilde{\Lambda}_{CP} = \tilde{\Lambda}_{PT}\Big|_{e_N} = 0$$

and T^1_{PT}, T^1_{PP}, T^1_{CP}, T^2_{PT}, T^2_{PP} and T^2_{CP} are well behaved functions of $\vec{p}_1$, $\vec{p}_2$ and $\vec{p}_1'$ which satisfy

$$T^1_{PT}\Big|_{E_f=E_i} = T^1_{PP}\Big|_{E_f=E_i} = T^1_{CP}\Big|_{E_f=E_i} = \langle\vec{p}_1,\vec{p}_2|S|\vec{p}_1'\rangle_{E_f=E_i}$$

and

$$T^2_{PT}\Big|_{E_f=E_i} = T^2_{PP}\Big|_{E_f=E_i} = T^2_{CP}\Big|_{E_f=E_i} = 0.$$

A similar singularity structure has been conjectured by Veselova [12] for the full off-shell T-matrix.

Under the appropriate smoothness assumptions it is not hard to see that (6.1), (6.2) and (6.3) satisfy (5.2) due to the oscillatory behavior of the singular factors as $E_f - E_i \to 0$. The substitution $E_f - E_i = \varepsilon u$, $u \in R^1$, allows one to show that the oscillations of the stationary renormalization terms in the definition of the renormalized half-shell T-matrices cancel the

oscillations of the singular factors in (6.1), (6.2) and (6.3) so that (5.4) is satisfied.

7 An Approximate Ionization S-matrix

In order to calculate the physical ionization S-matrix via the prior form of the half-shell T-matrix one requires the three particle wave function $\psi_-(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)$. This wave function does not satisfy the usual three particle integral equations due to the long-range nature of the Coulomb potential. In this section we discuss an approximate three particle wave function [17] which leads to an approximate expression for the ionization S-matrix. This approximation is justified via the time-dependent theory of Coulomb scattering and is independent of the existence of integral equations for $\psi_-(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)$.

The time-dependent theory has been used to verify the following [17]

$$\lim_{e\to 0} e^{-\beta}\left(\psi_-(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) - \psi_-^{app.}(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)\right) = 0,\ \beta < 4 \qquad (7.1)$$

in the sense of distributions where

$$\begin{aligned}\psi_-^{app.}(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) &= \phi_0(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)\\ &- \{\phi_0(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) - \psi_-(\vec{x}_1,\vec{p}_1)\phi_0(\vec{x}_2,\vec{p}_2)\}\\ &- \{\phi_0(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) - \psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1)\} \qquad (7.2)\\ &- \left\{\phi_0(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) - \psi_-\left(\vec{x}_1-\vec{x}_2,\ \frac{m_2\vec{p}_1-m_1\vec{p}_2}{m_1+m_2}\right)\phi_0\left(\frac{m_1\vec{x}_1+m_2\vec{x}_2}{m_1+m_2},\ \vec{p}_1+\vec{p}_2\right)\right\}\end{aligned}$$

where $\phi_0(\vec{x}_i,\vec{p}_i) = (2\pi)^{-3/2}\exp(i\vec{p}_i\cdot\vec{x}_i)$, $i = 1,2$ and $\phi_0(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) = \phi_0(\vec{x}_1,\vec{p}_1)\,\phi_0(\vec{x}_2,\vec{p}_2)$. The result (7.1) suggests that $\psi_-^{app.}(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)$ is a valid approximation to $\psi_-(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)$ for weak coupling

constants or from a physical viewpoint for sufficiently high momenta.

Replacing ψ_- by $\psi_-^{app.}$ in the expression for the prior half-shell T-matrix yields the following approximate physical S-matrix

$$\pi^{-1}\int d\vec{x}_1 d\vec{x}_2\ \overline{\psi_-^{app.}(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2)}\ \{V_{12}+V_1\}\ \phi_0(\vec{x}_1,\vec{p}_1)\phi_\alpha(\vec{x}_2)\Big|_{E_f=E_i} \tag{7.3}$$

The usual Born approximation for ionization [10] can be obtained from the prior form of the half-shell T-matrix by replacing ψ_- by $\psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1)$. It is not hard to see from (7.1) that

$$\lim_{e\to 0} e^{-\beta}\{\psi_-(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) - \psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1)\} \neq 0 \tag{7.4}$$

for $2 \leq \beta < 4$ and thus for small coupling constant $\psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1)$ is not as good an approximation to ψ_- as is $\psi_-^{app.}$. Clearly the approximation of ψ_- by $\psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1)$ does not treat all three final channel particles in a symmetric fashion.

We now give a formal justification of the Born approximation for ionization (7.3). If we assume that the incident particle 1 has a high final state energy compared to particle 2, i.e., $|\vec{p}_1| >> |\vec{p}_2|$ then from (7.2) we have

$$\psi_-^{app.}(\vec{x}_1,\vec{x}_2;\vec{p}_1,\vec{p}_2) \approx \psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1). \tag{7.5}$$

Substituting $\psi_-(\vec{x}_2,\vec{p}_2)\phi_0(\vec{x}_1,\vec{p}_1)$ for $\psi_-^{app.}$ in (7.3) yields the usual Born approximation. When both $|\vec{p}_2| \approx |\vec{p}_1|$ are large we expect that the Born approximation should be replaced by (7.3).

We now consider the particular scattering problem of ionization of hydrogen via electrons. We denote the approximate direct on-shell S-matrix (7.3) by $f(\vec{p}_1,\vec{p}_2)$. The approximate exchange on-shell S-matrix denoted by $g(\vec{p}_1,\vec{p}_2)$ is given by

$$g(\vec{p}_1,\vec{p}_2) = \int d\vec{x}_1 d\vec{x}_2\ \psi_-^{app.*}(\vec{x}_2,\vec{x}_1;\vec{p}_1,\vec{p}_2)\ \{V_{12}+V_1\}\ \phi_0(\vec{x}_1,\vec{p}_1)\phi_\alpha(x_2)\Big|_{E_f=E_i} \tag{7.6}$$

where $\psi_-^{app.*}(\vec{x}_2,\vec{x}_1;\vec{p}_1,\vec{p}_2)$ is obtained from (7.2) by interchanging $\vec{x}_1$ and $\vec{x}_2$. Since the approximate final channel wave function (7.2) treats the three particles in a symmetric fashion we have $f(\vec{p}_1,\vec{p}_2) \approx g(\vec{p}_2,\vec{p}_1)$ [8].

The above discussion shows that the approximation for the ionization scattering amplitude given by (7.3) and (7.6) satisfies the usual theoretical requirements. The computational usefulness of this approximation has not been examined.

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SCATTERING THEORY WITH LONG RANGE COULOMB POTENTIALS

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A summary is given of the mathematical analysis required for Coulomb scattering. A more general formulation is obtained on rotating the contour used to define the Whittaker function. A simple model for electron-ion scattering is considered. The analytical properties of a scattering matrix S_I are obtained in the complex momentum plane.

1 Introduction

Cross sections for electron impact excitation of positive ions are required for the interpretation of astronomical spectra. For lighter ions (for example O^{++}) they can be computed to an accuracy of about 5 percent, but such computations are expensive. Complicated resonance structures in the cross sections can be analyzed using quantum defect theory [1] which provides economic computational techniques. The method has a number of other applications, and may be of interest to specialists in mathematical scattering theory. In the present talk I describe some recent advances [2] in the mathematical foundations of the theory.

2 The Coulomb Radial Equations

The equation is

$$\left\{\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2Z}{r} + k^2\right\} y = 0 \quad . \tag{1}$$

Let us put

$$Zr = \rho \quad , \quad \left(\ell + \frac{1}{2}\right) = \lambda \quad , \quad (k/Z)^2 = \epsilon = -\frac{1}{\kappa^2} \quad . \tag{2}$$

Then

$$\left\{\frac{d^2}{d\rho^2} - \frac{\left(\lambda^2 - \frac{1}{4}\right)}{\rho^2} + \frac{2}{\rho} - \frac{1}{\kappa^2}\right\} y = 0 \quad . \tag{3}$$

Let us introduce the complex variable

$$z = 2\rho/\kappa \tag{4}$$

(for real positive energies $z = 2ikr$). Let $Y(\kappa,\lambda,z)$ be a solution of (3). Since λ and κ enter (3) only as λ^2 and κ^2, it follows that $Y(\kappa,-\lambda,z)$ and $Y(-\kappa,\lambda,-z)$ must also be solutions.

In the mathematical theory, one can treat λ and κ to be any complex numbers. I take ρ to be real and positive but this condition can be relaxed (as in co-ordinate rotation methods).

3 The Whittaker Function $M_{\kappa,\lambda}(z)$

Equation (3) has a solution

$$y_1(\kappa,\lambda;\rho) = \frac{\kappa^{\lambda+\frac{1}{2}}}{\Gamma(2\lambda+1)} M_{\kappa,\lambda}(z)$$

$$= \frac{\kappa^{\lambda+\frac{1}{2}}}{\Gamma\left(\lambda+\frac{1}{2}-\kappa\right)} z^{\lambda+\frac{1}{2}} e^{-z/2} \sum_{n=0}^{\infty} \frac{\Gamma\left(\lambda+\frac{1}{2}-\kappa+n\right) z^n}{\Gamma(2\lambda+1+n)n!} \quad . \tag{5}$$

In (5) one can expand $e^{-z/2}$ and re-arrange the series to give

$$y_1(\kappa,\lambda;\rho) = \sum_{m=0}^{\infty} \varepsilon^m y_{1,m}(\lambda;\rho) \tag{6}$$

which is absolutely and uniformly convergent: hence y_1 is an analytic function of ε.

It is well known in the theory of Coulomb scattering that y_1 can be expressed as a contour integral [3]. I will not go into all the details. The first step is to use the contour integral for the Γ function:

$$\frac{1}{\Gamma(2\lambda+1+n)} = \frac{1}{2\pi i}\int_{\infty e^{-i\pi}}^{(0+)} e^{t}\, t^{-2\lambda-1-n}\, dt \qquad (7)$$

where the contour starts at $\infty e^{-i\pi}$, encircles the origin and ends at $\infty e^{+i\pi}$. Substitution of (7) in (5) gives an expansion in (z/t) which can be summed by the binomial theorem if $|z/t| < 1$. This condition is satisfied if we make a suitable deformation of the contour, and assume

$$|\arg(z)| < \pi \quad . \qquad (8)$$

One obtains

$$y_1 = \frac{\kappa^{\lambda+\frac{1}{2}}}{2\pi i}\, z^{\lambda+\frac{1}{2}}\, e^{-z/2} \int_{C'} e^{t}\, t^{-\lambda-\frac{1}{2}-\kappa}\, (t-z)^{-\lambda-\frac{1}{2}+\kappa}\, dt \qquad (9)$$

where C' starts at $\infty e^{-i\pi}$, encircles the points $t = 0$ and $t = z$, and ends at $\infty e^{+i\pi}$. One can now make further deformations of the contour so as to express y_1 in terms of two integrals of the type

$$\int_{\infty e^{-i\pi}}^{(0+)} \ldots\, dt \quad .$$

4 The Whittaker Function $W_{\kappa,\lambda}(z)$

Whittaker's definition of the function $W_{\kappa,\lambda}(z)$ (which is a solution of (3)) is

$$W_{\kappa,\lambda}(z) = \frac{\Gamma\left(\kappa+\frac{1}{2}-\lambda\right)}{2\pi i}\, e^{-z/2}\, z^{\kappa} \int_{\infty e^{-i\pi}}^{(0+)} e^{t}\, t^{\lambda-\frac{1}{2}-\kappa} \left(1-\frac{t}{z}\right)^{\lambda-\frac{1}{2}+\kappa} dt$$

$$\text{for } |\arg(z)| < \pi \quad . \qquad (10)$$

Expansion of $(1-t/z)$ gives the asymptotic form

$$W_{\kappa,\lambda}(z) \underset{|z|\to\infty}{\sim} z^{\kappa} e^{-z/2} \quad . \tag{11}$$

The function $y_1(\kappa,\lambda;z)$ can be expressed in terms of $W_{\kappa,\lambda}(z)$ and $W_{-\kappa,\lambda}(-z)$.

It is at this point that a difficulty arises for the case of the attractive Coulomb field ($Z > 0$). If ε is real and negative we have $|\arg(z)| = \pi$ or $|\arg(-z)| = \pi$, so that the condition (8) is violated for one of the Whittaker functions. The difficulty is overcome on rotating the contour in (10) through an angle β, i.e., to

$$\int_{\infty e^{-i(\pi+\beta)}}^{(0+)} \ldots \, dt \tag{12}$$

where β must be such that

$$\left.\begin{aligned} -\frac{\pi}{2} < \beta < +\frac{\pi}{2} \\ -(\pi+\beta) < \arg(z) < (\pi-\beta) \end{aligned}\right\} \tag{13}$$

(these conditions are not given correctly in some standard textbooks). For any value of z such that

$$|\arg(z)| < \frac{3\pi}{2} \tag{14}$$

we can find a value of β satisfying (13) and hence define $W_{\kappa,\lambda}(z)$ over the more extended range (14) of arg(z).

5 Relations Between the Functions $M_{\kappa,\lambda}(z)$ and $W_{\kappa,\lambda}(z)$

We must be careful about the meaning of (-z); we put $(-z) = e^{i\pi D} z$ with $D = +1$ or $D = -1$. The expression for y_1 in terms of Whittaker functions is then

$$y_1(\kappa,\lambda;\rho) = \kappa^{\lambda+\frac{1}{2}}\, e^{i\pi\kappa D}$$

$$\times \left\{ \frac{e^{-i\pi\left(\lambda+\frac{1}{2}\right)D} W_{\kappa,\lambda}(z)}{\Gamma\left(\kappa+\lambda+\frac{1}{2}\right)} + \frac{W_{-\kappa,\lambda}(e^{i\pi D}z)}{\Gamma\left(-\kappa+\lambda+\frac{1}{2}\right)} \right\} \qquad (15)$$

where we can take $D = +1$ for $-3\pi/2 < \arg(z) < \pi/2$ or $D = -1$ for $-\pi/2 < \arg(z) < +3\pi/2$. From (15) and (11) we obtain the asymptotic form of y_1.

6 Two Solutions Analytic in ε

The functions $y_1(\kappa,\lambda;\rho)$ and

$$y_2(\kappa,\lambda;\rho) = y_1(\kappa,-\lambda;\rho) \qquad (16)$$

are solutions of (3) analytic in ε, but for $\lambda = (\ell+\frac{1}{2})$ they are not linearly independent. The relationship between them is

$$y_2 = -A\, y_1 \quad \text{for} \quad \lambda = (\ell+\tfrac{1}{2}) \qquad (17)$$

where

$$A(\kappa,\lambda) = \frac{\Gamma\left(\kappa+\lambda+\frac{1}{2}\right)}{\kappa^{2\lambda+1}\,\Gamma\left(\kappa-\lambda+\frac{1}{2}\right)} \quad . \qquad (18)$$

A third solution may be defined as

$$y_3 = \frac{A\cos(2\pi\lambda)y_1 - y_2}{\sin(2\pi\lambda)} \quad . \qquad (19)$$

In (19) we may take the limit $\lambda \to \ell+\frac{1}{2}$. This gives a term in

$$G = \frac{1}{2\pi}\frac{\partial}{\partial\lambda} A\Big|_{\lambda=\ell+\frac{1}{2}} \qquad (20)$$

which is not analytic in ε. Subtracting this term we have

$$y_4 = y_3 - G\, y_1 \tag{21}$$

which is analytic in ε for $\kappa = \ell + \frac{1}{2}$.

Changing notation, we take the two solutions analytic in ε, for $\lambda = \ell + \frac{1}{2}$, to be

$$\left.\begin{aligned} f(\varepsilon,\ell;\rho) &= y_1\left(\kappa,\ell+\tfrac{1}{2},\rho\right) \\ g(\varepsilon,\ell;\rho) &= y_4\left(\kappa,\ell+\tfrac{1}{2};\rho\right) \end{aligned}\right\} \quad . \tag{22}$$

The regular solution (zero at the origin) is f, and the irregular solution is g.

7 The Collision Problem

In a rigorous treatment, the electron-ion collision problem must be treated as a many-body problem with all electrons indistinguishable. For this problem it is difficult to formulate any rigorous theorems. I will therefore consider a simple model problem which corresponds to non-exchange close coupling with potentials (other than Coulomb potentials) of finite range. For this problem we have a set of coupled differential equations

$$\left\{\frac{d^2}{d\rho^2} - \frac{\ell_i(\ell_i+1)}{\rho^2} + \frac{2}{\rho} + \varepsilon_i\right\} F_i(\rho) + \sum_j U_{ij}(\rho) F_j(\rho) = 0 \tag{23}$$

where

$$\varepsilon_i = (E-E_i)/Z^2 \tag{24}$$

and where E is the total energy, E_i the energy of target state i. In a more compact matrix notation,

$$\left(\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{2}{\rho} + \varepsilon + U\right) F = 0 \quad . \tag{25}$$

We take $U(\rho)$ to be such that

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$$U(\rho) = 0 \quad \text{for} \quad \rho > \rho_1 \quad \text{with} \quad \rho_1 < \infty \quad . \tag{26}$$

We consider only solutions of (25) which are zero at the origin,

$$F(\rho=0) = 0 \quad . \tag{27}$$

8 Solutions Analytic in E

The potential matrix $U(\rho)$ is such that (25) has solutions $F(E,\rho)$ satisfying

$$\lim_{\rho\to 0} \left\{\rho^{-\ell-1} F(E,\rho)\right\} = 1 \quad . \tag{28}$$

This condition is independent of E. Solutions $F(E,\rho)$ satisfying (28) are analytic in E for all finite ρ [4]. For $\rho > \rho_1$ they are linear combinations of f and g:

$$F(E,\rho) = f(\varepsilon,\ell;\rho)I(E) + g(\varepsilon,\ell;\rho)J(E) \quad \text{for} \quad \rho > \rho_1 \quad , \tag{29}$$

and the coefficient matrices I(E) and J(E) are analytic in E.

9 The Scattering Matrix S_I

Let us define

$$\left.\begin{aligned} \phi^{+} &= (\kappa/i)^{1/2}\, e^{i\frac{\pi}{2}(\kappa-\ell)}\, W_{\kappa,\ell+\frac{1}{2}}(z) \\ \phi^{-} &= (\kappa/i)^{1/2}\, e^{-i\frac{\pi}{2}(\kappa-\ell)}\, W_{-\kappa,\ell+\frac{1}{2}}(e^{i\pi}z) \end{aligned}\right\} \quad . \tag{30}$$

For the case of ε real we may put $\kappa = i\gamma$ for $\varepsilon > 0$ and $\kappa = \nu$ for $\varepsilon < 0$, with γ and ν real and positive. We then have, for $|z| \to \infty$,

$$\phi^{\pm} \sim \begin{cases} \gamma^{1/2} \exp\left\{\pm i\left[\frac{\rho}{\gamma} - \frac{\pi}{2}\ell + \gamma\, \ell n\left(\frac{2\rho}{\gamma}\right)\right]\right\} & \text{for} \quad \kappa = i\gamma \\ \left(\frac{\nu}{i}\right)^{1/2} \exp\left\{\pm\left[-\frac{\rho}{\nu} - \frac{\pi i}{2}(\ell-\nu) + \nu\, \ell n\left(\frac{2\rho}{\nu}\right)\right]\right\} & \text{for} \quad \kappa = \nu \end{cases} . \tag{31}$$

For $\varepsilon > 0$, ϕ^+ and ϕ^- correspond to outgoing and incoming spherical waves.

Equations (25) have solutions $F(S_I,\rho)$ such that

$$F(S_I,\rho) = \phi^- - \phi^+ S_I \quad \text{for} \quad \rho > \rho_1 \tag{32}$$

which defines S_I [5].

10 Analytical Structure of S_I

We may express ϕ^-, ϕ^+ in terms of f and g, and hence express $F(S_I,\rho)$ in terms of $F(E,\rho)$ and S_I in terms of I(E) and J(E). The final result is

$$S_I = \frac{\kappa^{\ell+\frac{1}{2}} \exp\left[i\frac{\pi}{2}(\kappa-\ell)\right]}{\Gamma(\kappa+\ell+1)} \times [I - (iA+G)J][I - (A\cot(\pi\kappa)+G)J]^{-1} \times \frac{\Gamma(-\kappa+\ell+1)}{\kappa^{\ell+\frac{1}{2}} \exp\left[i\frac{\pi}{2}(\kappa-\ell)\right]}, \tag{33}$$

$$\text{for} \quad -\frac{\pi}{2} < \arg(\kappa) < +3\frac{\pi}{2} \quad .$$

This is my main new result. It gives S_I in terms of known functions of κ, and of I and J, the analytical functions of E. Previous work [5] gave S_I only for E real.

11 Some Special Cases

(i) Pure Coulomb scattering. With $U(\rho) = 0$ we have $J = 0$ and

$$S_I = \Gamma(-\kappa+\ell+1)/\Gamma(\kappa+\ell+1) \quad . \tag{34}$$

This result is well known [6].

For ε real and positive (34) gives $S_I = \exp(2i\sigma)$ with $\sigma = \arg\Gamma(\ell+1-i\gamma)$. We have $\varepsilon = 1/\gamma^2$ and hence $\gamma \to \infty$ as $\varepsilon \to 0$.

For γ large, we have $\sigma \to \gamma[1 - \ell n(\gamma)]$ from Stirling's formula. Thus S_I has infinite oscillations in the limit of $\varepsilon \to 0$.

For ε real and negative we have $\varepsilon = -1/\nu^2$; S_I has poles at the poles of $\Gamma(-\nu+\ell+1)$, i.e., at $\nu = n$ with $n = (\ell+1),(\ell+2),\ldots$. These are the bound states.

(ii) The one-channel problem. With one equation but $U(\rho) \neq 0$ for $\rho < \rho_1$ we have $J \neq 0$. For this case we find that

$$S_I = \exp\{2i[\sigma + \pi\mu(\varepsilon)]\} \quad \text{for} \quad \varepsilon > 0 \tag{35}$$

and that S_I has poles at $\nu = n-\mu(\varepsilon)$ for $\varepsilon < 0$. The quantum defect, $\mu(\varepsilon)$, can be expressed in terms of I(E) and J(E). To employ an expression used by several other speakers, $\mu(\varepsilon)$ is a "nice" function. For practical purposes it can usually be fitted to a low order polynomial in ε. It can be expressed in terms of known functions of κ and analytical functions of ε but is not itself an analytic function of ε.

(iii) The many-channel problem. When some channels are open ($Re\ \varepsilon_i > 0$) and some closed ($Re\ \varepsilon_j < 0$), S_I has poles at complex energies below the real energy axis. These poles form sequences with points of accumulation at thresholds, $\varepsilon_i = 0$.

12 Computational Procedures

The matrix S_I is not used in computational work. For all channels open we may define a matrix

$$\chi = e^{-i\sigma}\, S_I\, e^{-i\sigma} \tag{36}$$

which is "nice" in that it can be extrapolated smoothly to the region of some channels closed. In this region it can be partitioned according to the scheme

$$\chi = \begin{pmatrix} \chi_{oo} & \chi_{oc} \\ \chi_{co} & \chi_{co} \end{pmatrix} \begin{matrix} \text{open} \\ \text{closed} \end{matrix} \qquad (37)$$

$$\text{open} \quad \text{closed}$$

The scattering matrix S from the computer corresponds to functions F with asymptotic form

$$F_{ij} \sim \begin{cases} \gamma_i^{1/2} \left\{ e^{-i\zeta_i} \delta_{ij} - e^{+i\zeta_i} S_{ij} \right\} & \text{for} \quad \varepsilon_i > 0 \\ 0 \quad \text{for} \quad \varepsilon_i < 0 \quad , \end{cases} \qquad (38)$$

where

$$\zeta = \frac{\rho}{\gamma} - \frac{\pi}{2} \ell + \gamma \ln\left(\frac{2\rho}{\gamma}\right) + \sigma \quad . \qquad (39)$$

The relation between S and χ is

$$S = \chi_{oo} - \chi_{oc} \left\{ \chi_{cc} - e^{-2\pi i \nu_c} \right\}^{-1} \chi_{co} \quad . \qquad (40)$$

This is the type of relation which can be used to obtain completely resolved resonance profiles from computations made at a fairly small number of energies.

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NONSINGULAR VARIATIONAL PRINCIPLE FOR THE SCATTERING LENGTH FOR THE TARGET WAVE FUNCTION IMPRECISELY KNOWN

Larry Spruch and Leonard Rosenberg

Abstract

Variational principles for the scattering length A for potential scattering, and for scattering by a compound target whose ground state energy ε and ground state wave function ϕ are known, have been available for some thirty years. These variational principles (VP's) are free of any singularities and associated numerical instabilities and will be referred to as nonsingular VPs. They are extremely useful where applicable, but in atomic and molecular physics they are largely limited to scattering by atomic hydrogen targets. They are reviewed from a perspective which is helpful in extending the VP to scattering by targets with imprecisely known ϕ and ε, for which the only available principle for A, until very recently, was a singular VP. (Most so called VP's in scattering theory are really singular VP's. The VP for A, for ϕ and ε known, is an exception; for that case one has a variational bound, which gives the sign of the error and guarantees that the VP is nonsingular.) We discuss a nonsingular VP for A, for ϕ and ε imprecisely known, which was very recently obtained and which has just been tested on a model problem, and a new nonsingular VP.

I. Introduction

Variational principles (VP's) in scattering theory were first developed in the 1940's by Schwinger, Kohn [10], and many others [11]. We begin with some terminology.

An estimate $Q_{st} = Q_{st}(w_t)$ of the quantity $Q = Q(w)$ to be determined will be referred to as a stationary principle if the error $Q_{st} - Q$ is of order $(\delta w)^2$, where $\delta w \equiv w_t - w$ is the error in the input function w_t, a guess at the true function w. (More

generally, w can represent a set of unknown functions and a set of unknown constants.) An estimate Q_{var} will be referred to as a VP if, for any reasonable <u>form</u> of w_t, with linear or nonlinear parameters in w_t determined by setting the variation of w_t with respect to them equal to zero, the w_t (and the Q_{var}) so determined is reasonable. With the above definition, most so called VP's in scattering theory, where w is the unknown scattering wave function, are not truly VP's; there can be values of the nonlinear parameters for which, using a so-called VP, the estimate thereby obtained will be very bad or even infinite, even for a trial function of a very reasonable form. We will refer to such a so-called VP as a singular VP. Singular VP's can be and have been extremely useful, but they can be the source of very confusing numerical instabilities and it is clearly much preferable, where possible, to have a true VP.

We will now elaborate on the above remarks, beginning with a discussion of scattering by a potential, and by a compound target with a known associated energy ε. One normally uses singular VP's for an incident kinetic energy $E \neq 0$, but for $E = 0$ one has available a simple nonsingular VP. Although this case has been treated extensively in the literature [17], we will review it nevertheless, but briefly, and from a point of view which might suggest how to proceed when ϕ is imprecisely known.

A. <u>Potential Scattering</u>

We consider scattering by a short-ranged central potential, V(q). The exact scattering wave function $\omega(q)$ for $E = k^2\hbar^2/2m \neq 0$ and zero orbital angular momentum is finite at $q = 0$ and satisfies

$$(T + V - E)\omega = 0 \ , \tag{1.1}$$

where T is the kinetic energy operator, and the boundary condition (bc)

$$\omega \sim (\sin kq + \tan \eta \cos kq)/q \ , \quad q \sim \infty \ , \tag{1.2}$$

where η is the $\ell = 0$ phase shift. We introduce a trial function ω_t which is finite at the origin and satisfies the same bc as does ω, but with η replaced by a trial phase shift η_t, and we work in units in which

$$C \equiv 4\pi(\hbar^2/2m) \tag{1.3}$$

is equal to unity. The Kohn estimate for k tan η is given by

$$(k \tan \eta)_K = k \tan \eta_t - (\omega_t, (T + V - E)\omega_t) , \tag{1.4}$$

where the volume element in the inner product is $4\pi q^2\, dq$. If the error function $\delta\omega \equiv \omega_t - \omega$ is small, the Kohn estimate will be in error by a quantity of order $(\delta\omega)^2$ and is therefore a stationary principle. If, however, ω_t is a sum of N basis functions each multiplied by an arbitrary constant -- a linear variational parameter -- the determination of these parameters requires the inversion of the N by N matrix whose elements are the matrix elements of the operator T + V - E formed with the N basis functions. E lies within the continuous spectrum of T + V, and while it is possible to define the inverse of T + V - E to be finite for $N = \infty$, no such definition seems to be possible for any finite value of N, so that the inverse can be "nearly singular" or even singular for any finite value of N. The Kohn estimate is therefore a singular VP. Some of the detailed effects of these singularities have been studied [3,15] but they will not concern us.

The situation is far simpler for E = 0. The exact scattering length A is defined as the limit as $k \sim 0$ of $-\tan \eta/k$. The exact E = 0 scattering wave function ψ is finite at q = 0, and satisfies $(T + V)\psi = 0$ and the bc

$$\psi \sim (q - A)/q , \quad q \sim \infty . \tag{1.5}$$

We introduce a trial scattering function ψ_t which is finite at q = 0 and behaves asymptotically as

$$\psi_t \sim (q - A_t)/q , \quad q \sim \infty , \tag{1.6}$$

where A_t is a trial scattering length. For later reference we note that

$$\delta\psi \sim -(A_t - A)/q \equiv -\delta A/q \ , \quad q \sim \infty \ . \tag{1.7}$$

The Kohn estimate of A is then

$$A_K = A_t + (\psi_t, (T + V)\psi_t)/C \ , \tag{1.8}$$

where C, defined by Eq. (1.3), will be dropped and must henceforth be understood. To simplify the discussion, we assume that there are no bound states. As opposed to $(k \tan \eta)_K$, the estimate A_K is a VP; there are no possible singularities. The essential difference from the $E \neq 0$ case is simply that the eigenvalue zero lies at the edge rather than in the middle of the continuum eigenvalue spectrum of T + V. That there is such an essential difference is suggested by the more sophisticated approach required to define the *integral in momentum space* $\hbar \vec{k}'$ which gives the coordinate representation of the inverse of T + V - E for $E \neq 0$ than for E = 0; in the former case one must distort the contour or use the $\pm i\varepsilon$ formalism to avoid the singularity at k' = k associated with the denominator $(k')^2 - k^2$, but for E = k = 0 the $(k')^2$ in the denominator is cancelled by the $(k')^2$ in d^3k'.

A_K is not only a VP for A but a variational bound (V Bd) on A; it is an upper V Bd. Thus, we replace Eq. (1.8) by the identity

$$A = A_t + (\psi, (T + V)\psi_t) = A_t + (\psi_t, (T + V)\psi_t) - (\delta\psi, (T + V)\psi_t)$$

$$= A_K - (\delta\psi, (T + V)\,\delta\psi) \ . \tag{1.9}$$

It follows from the assumption of no bound states and the Rayleigh-Ritz theorem that the expectation value of T + V is nonnegative for any quadratically integrable function and, more generally [16], for a function such as $\delta\psi$ which behaves as (constant/q) as $q \sim \infty$. The upper V Bd property of A_K follows immediately. While A_K can therefore never be arbitrarily large and negative (unless A is), A_K can be arbitrarily large and posi-

tive, though only for an unrealistic ψ_t , such as one which oscillates extremely rapidly. It is to be noted that an upper V Bd not only gives an estimate good to second order, with an error of known sign, but guarantees that there will be no singularity of the type normally encountered in which the estimate can take on arbitrarily large positive and negative values.

Though it can be of little significance in potential scattering, we record what seems to be a new identity for A because it may may be useful for more complicated scattering problems. We introduce a trial function of the form

$$\psi_{tt}(q) \sim 1 - A_t \exp(-\kappa q)/q + \cdots ,$$

where the unrecorded terms fall off much faster than the $\exp(-\kappa q)$ term. ψ_{tt} does not have the same asymptotic form as ψ, but if κ is sufficiently small it need differ from ψ only in the region of large q where the potential is in any event negligible. We then find, rather than Eq. (1.9), the identity

$$A = (\psi, (T + V)\psi_{tt}) . \tag{1.10}$$

The A_t term is not present; it arose from a surface term which no longer contributes since $d\psi_{tt}/dq$ vanishes rapidly as $q \to \infty$.

It will be useful for later purposes to derive an equivalent but alternative form for A_K. Writing ψ and ψ_t in forms which isolate their asymptotic value, 1, we have

$$\psi = 1 + p(q) \sim 1 - (A/q) , \quad \psi_t = 1 + p_t(q) \sim 1 - (A_t/q). \tag{1.11}$$

Using Eq. (1.11) and $(1,T\psi_t) = - A_t$, which follows on integrating by parts, Eq. (1.8) becomes

$$A_K = (1,V1) + 2(1,Vp_t) + (p_t,(T + V)p_t) . \tag{1.12}$$

B. Scattering by a Compound Target with a Known Ground State Wave Function ϕ

We turn now to scattering by a compound system. The target

hamiltonian will be denoted by $h(\vec{r})$, where $\vec{r}$ represents all internal coordinates, and we have

$$h\phi = \varepsilon\phi \ , \quad (\phi,\phi) = 1 \ . \tag{1.13}$$

It will suffice to consider i) an infinitely massive target and ii) an interaction $V(\vec{r},\vec{q})$ between the incident particle and the target which is a sum of short-ranged central two-body interactions. We further assume iii) that the ground state is spherically symmetric, which we represent symbolically by writing $\phi(r)$ rather than $\phi(\vec{r})$, iv) that spin interactions are negligible, v) that the incident particle is distinguishable, and vi) that there are no composite bound states. The hamiltonian H of the system comprising the target and the incident particle is then

$$H(\vec{r},\vec{q}) = h(\vec{r}) + T + V(\vec{r},\vec{q}) \ . \tag{1.14}$$

The Kohn estimate of η, an extension of Eq. (1.4), will be a singular VP, since the total energy lies in the continuum of H, and we consider only $k = 0$. The expressions we seek are trivial extensions from the potential scattering case. The exact scattering wave function Ψ is finite at $q = 0$, and satisfies $(H - \varepsilon)\Psi = 0$ and the bc

$$\Psi(\vec{r},\vec{q}) \sim \phi(r)(q - A)/q \ , \quad q \sim \infty \ . \tag{1.15}$$

The trial function Ψ_τ will be chosen to be finite at $q = 0$ and to behave asymptotically as

$$\Psi_\tau(\vec{r},\vec{q}) = \sim\phi(r)(q - A_t)/q \ , \quad q \sim \infty \ . \tag{1.16}$$

We then have

$$A_K = A_t + (\Psi_\tau, (H - \varepsilon)\Psi_\tau) \tag{1.17}$$

as a VP for A; there are no singularity difficulties since ε lies at the edge of the continuum of H. In fact, A_K is not simply a VP but an upper V Bd.

If we extract the asymptotic component ϕ by introducing the scattered component $F = F(\vec{r},\vec{q})$ of Ψ and writing

$$\Psi = \phi + F \sim \phi(q - A)/q \ , \quad \Psi_\tau = \phi + F_\tau \sim (q - A_t)/q \ ,$$

Eq. (1.17) becomes

$$A_K = \left(\phi,(H - \varepsilon)\phi\right) + 2\left(F_\tau,(H - \varepsilon)\phi\right) + \left(F_\tau,(H - \varepsilon)F_\tau\right). \qquad (1.18)$$

II. A Singular VP for A, for ϕ Imprecisely Known

We now consider zero incident energy scattering by a compound target for which ϕ and ε are only imprecisely known. We make the same six assumptions as were listed below Eq. (1.13). We introduce a normalized trial function $\phi_t(r)$ with parameters chosen to minimize

$$\varepsilon_t \equiv (\phi_t, h\phi_t) \ ,$$

and note that $\varepsilon_t \geq \varepsilon$; *no changes in* ϕ_t will be made in the course of the analysis of the scattering problem.

Ψ and F are of course still defined as above, but since ϕ is not known we must alter the forms of Ψ_τ and F_τ to forms to be denoted by Ψ_t' and F_t' , respectively. The most obvious choice -- but by no means the only choice, as we will see -- is

$$\Psi_t' = \phi_t + F_t' \sim \phi_t(q - A_t)/q \ . \qquad (2.1)$$

It is then natural, in replacing the Kohn forms (1.17) and (1.18), to consider the expressions

$$A_D = A_t + (\Psi_t', (H - \varepsilon_t)\Psi_t') \qquad (2.2a)$$

$$= (\phi_t,(H - \varepsilon_t)\phi_t) + 2(F_t',(H - \varepsilon_t)\phi_t) + (F_t',(H-\varepsilon_t)F_t') \qquad (2.2b)$$

If one makes the choice Ψ_t' and F_t' given by (2.1) and if one attempts to mimic Eqs. (1.17) and (1.18), one must replace ε by ε_t, for the replacement of ε by $\varepsilon' \neq \varepsilon_t$ would cause the term $(\phi_t,(h - \varepsilon')\phi_t)$ that would appear in A_D to diverge at large q.

Remarkably, as first shown by Demkov [4], the simple form (2.2a) is a stationary principle -- $A_D - A$ is of second order in *all* errors, including $\delta\phi = \phi_t - \phi$. (The form (2.2b) will then also be stationary.) The form (2.2a) is often referred to as a VP, but it is clear that in our terminology it is a singular VP, since ϵ_t lies within the continuous spectrum of H. The form (2.2a) has been studied in some model problems [9,12,13], and as is to be expected on the basis of the above discussion it gave rise to very troublesome numerical instabilities.

The obvious extension of (2.2a) to $E \neq 0$ was shown by Demkov to represent a stationary principle for η. That extension is also a singular VP, but the elimination of the singular nature of the VP is far more difficult for $E \neq 0$ than for $E = 0$, and we limit the major part of our discussion to the latter case. (We remark, incidentally, that the stationary property of the Demkov principle is lost for scattering energies in the neighborhood of a threshold for excitation of the target. This can be related to the existence of singularities in the scattering amplitude as a function of energy in those threshold regions.)

III. A Nonsingular VP for A, for ϕ Imprecisely Known

We can rewrite Eq. (2.2a) as

$$A_D = a' + 2b' + c',$$

where

$$a' \equiv (\phi_t, (H-\epsilon_t)\phi_t) = (\phi_t, V\phi_t)$$

$$b' \equiv (F_t', (H-\epsilon_t)\phi_t)$$

$$c' \equiv (F_t', (H-\epsilon_t)F_t') \ .$$

To determine the linear parameters in F_t', one must insert the operator which appears in the term quadratic in F_t', the term c', and it is the inversion of $(H-\epsilon_t)$ which is the source of numeri-

cal instabilities and of the singular nature of the VP given by A_D. In an attempt to obtain a nonsingular VP [2], one might therefore, in the term c' and perhaps elsewhere, try to replace ε_t by $\tilde{\varepsilon}$, where $\tilde{\varepsilon}$ lies *below* ε (and therefore outside of the spectrum of H) and is good to second order. (A value of $\tilde{\varepsilon}$ might be provided theoretically by a lower V Bd on ε, or experimentally by the use of data. In the latter case, we will simply define $\tilde{\varepsilon}$ to be good to second order if the data are "sufficiently accurate".) If, however, we simply replace ε_t in c' by $\tilde{\varepsilon}$, the part of c' that is proportional to $(\phi_t f, (h-\tilde{\varepsilon})\phi_t f)$, where f(0) is finite, $f(q) \sim 1/q$ for $q \sim \infty$, is in turn proportional to (f,f), an integral in q space which is infinite. To be concrete, f will be taken to be $[1 - \exp(-\mu q)]/q$. One possible remedy -- others have not yet been explored -- is to leave ϕ_t as it is and to replace F_t' in c' by $F_t = F_t'S$, where S is a convergence factor in q space which we take to be $\exp(-\kappa q)$ where we define κ by

$$\kappa^2\hbar^2/2m = \varepsilon_t - \tilde{\varepsilon} \ .$$

(κ can be treated as a variational parameter [2], but we will not utilize that freedom.) (The introduction of S is not an unnatural step. Qualitatively, we have $\tilde{\varepsilon}$ below ε, and we know that for an energy *above* ε, Ψ contains a component which oscillates as a function of q for q large. Quantitatively, we have that

$$g(q) \equiv \int d\vec{r}\ \phi(r)\ (H - \varepsilon) \left\{-A\ \phi(r)/q\right\}$$

$$g_t(q) \equiv \int d\vec{r}\ \phi_t(r)\ (H - \varepsilon_t) \left\{-A_t\phi_t(r)/q\right\}$$

$$\tilde{g}(q) \equiv \int d\vec{r}\ \phi_t(r)\ (H - \tilde{\varepsilon}) \left\{-A_t\phi_t(r)\ \exp(-\kappa q)/q\right\}$$

all tend to zero as $q \sim \infty$, where the quantity in curly brackets is the asymptotic form of the scattered wave and approximations to it.) If, therefore, we introduce

$$c \equiv (F_t, (H - \tilde{\varepsilon})F_t) \ ,$$

we readily find that c is finite, that c remains finite as $\kappa \sim 0$, and that $\lim (c' - c) = 0$, where lim denotes the limit as κ goes to zero.

It is not necessary, but we consider the replacement of b'. A first guess might be $b'' \equiv (F_t, (H - \tilde{\varepsilon})\phi_t)$, but $\lim (b'' - b') \neq 0$ and it seems more reasonable to choose

$$b \equiv (F_t, V\phi_t) ,$$

which is finite, remains finite as $\kappa \sim 0$, and satisfies $\lim (b'-b) = 0$. (Note that $b'' - b = (F_t, (h-\tilde{\varepsilon})\phi_t)$ is proportional to $(h-\tilde{\varepsilon})\phi_t$, which vanishes as $\kappa \sim 0$, but that nevertheless $\lim (b'' - b) \neq 0$; the point is that the integral over q diverges as $q \sim \infty$.) The first form of a' would suggest $(\phi_t, (H-\tilde{\varepsilon})\phi_t)$, but this is infinite, so we choose the second form for a'. We now have a form introduced by Blau and the present authors [2] -- arrived at by an entirely different route -- namely,

$$A_{BRS} = (\phi_t, V\phi_t) + 2(\phi_t, VF_t) + (F_t, (H-\tilde{\varepsilon})F_t) . \qquad (3.1)$$

This expression (i) is finite, (ii) remains finite as $\kappa \sim 0$, (iii) differs term by term from A_D by expressions which vanish as $\kappa \sim 0$, and (iv) enables one to determine the parameters in F_t in a singularity-free fashion. There is only one small problem; the expression is not variational with respect to the error $\delta\phi$ in ϕ_t! For a good ϕ_t, the result can nevertheless be useful. The expression (3.1) was used in a study of $e^{\pm}$ scattering by a hydrogen atom, with ϕ assumed to be imprecisely known [1]; as was to be expected, there were no singularities and no instabilities. We are presently using the trial wave function obtained in the Demkov form to obtain variationally accurate results. (Dropping S gives F_t'.)

We mention a more attractive possibility, one we have not yet fully examined. We write

$$F_t' = - A_t\phi_t(r)\, f(q) + \chi_t(r,q) ,$$

$$F_t = - A_t \phi_t f S + \chi_t \ ,$$

the convergence factor having been attached only to the dominant component of the scattered wave. It isn't really necessary to multiply χ_t by S since χ_t decays exponentially in q (and in r), and we want F_t to be as close as possible to F_t'. We then introduce a new estimate of A,

$$A_{SR} = a' + 2b' + c \ .$$

A_{SR} has the four advantages and the one disadvantage of A_{BRS} listed just above. Indeed, it is closer in form to A_D than is A_{BRS}. We have

$$\Delta \equiv A_D - A_{SR} = (F_t', (H-\epsilon_t)F_t') - (F_t, (H-\tilde{\epsilon})F_t) \ .$$

It should be possible to eliminate χ_t , the only complicated expression, since χ_t appears in the form $(H-\epsilon_t)\chi_t$ multiplied by a first order term, so that we can use

$$(H \epsilon_t)\chi_t \approx - (H-\epsilon_t)\phi_t(1 - A_t f) \ ,$$

and to express Δ as a simple readily calculable function of A_t , f, ϕ_t , H , ϵ_t and $\tilde{\epsilon}$, neglecting only second order terms. Thus, having obtained A_{SR} , in the course of which A_t is obtained, A_D is simply $A_{SR} + \Delta$. An elementary calculation gives

$$\Delta = 2\kappa A_t \{ A_t + (\phi_t [1 - \exp(-\mu q)], V\phi_t) \} \ .$$

IV. Discussion

We close with four comments.

(1) The essential achievement of the present paper was the conversion of a stationary principle involving an operator that is not of definite sign to a stationary principle involving a nonnegative operator. It would be interesting to see if there are other problems for which the same improvement could be made.

(2) It has been argued [6] that one should be able to

construct a VP for just about any well posed problem in mathematical physics by the use of undetermined Lagrange multipliers, but we have imposed two additional requirements in the present paper. The first, explicitly stated, is that we demand a true VP rather than a singular VP. The second, left tacit until now, is that we seek a VP for which we need not introduce additional trial functions, Lagrange multipliers. (We certainly don't want this new class of functions to be obtained by methods which are numerically unstable.) If we drop the second requirement, we can replace ϕ_t in (3.1) by a nonsingular VP for ϕ_t. If the additional effort seems worthwhile, the VP can be promoted to a V Bd, as discussed in [2].

(3) Singular VP's also arise in the estimation of a wide class of bound state matrix elements, including $(\phi,W\phi)$, where W is an arbitrary operator. The nature of the singularity is different from that considered in the present analysis of A, and more troublesome. In the present problem we simply shift from ε, at the edge of the continuum, or ε_t, within the continuum to $\tilde{\varepsilon}$, outside the continuum; the shift, and the low density of states in the immediate neighborhood of zero incident kinetic energy, generate a nonsingular VP. In the bound state case, the singularity originates in a denominator $\varepsilon_n - \varepsilon_{nt}$, so that, speaking schematically, the singularity is concentrated at a point, the discrete eigenvalue ε_n, and there is no density of states. The achievement of a nonsingular VP [7] required a modification of the Hamiltonian.

(4) An even more troublesome singularity arises in the analysis of scattering at $E \neq 0$, for then one lies in the middle of the continuum. In some unpublished work, one of us (LR) has used an effective potential approach [14] to generate a nonsingular VP, but attempts should be made to obtain a simpler version. One possible avenue of approach is the Feshbach projection operator approach [5]. This approach is one of the methods that has

been used [8] to obtain an upper V Bd -- which is better than a nonsingular VP -- for the phase shift, for ϕ known, and an attempt should be made to see if a similar attack enables one to extend the domain of applicability to the case for which ϕ is only imprecisely known. (By projecting onto a space of functions orthogonal to ϕ, for ϕ known, one in a sense eliminates the continuum associated with ϕ.) A less ambitious project would be to seek a nonsingular VP for the effective range, for ϕ only imprecisely known; this was done [17] for ϕ known by T. O'Malley and the present authors.

Acknowledgments

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APPLICATION OF ATOMIC SCATTERING THEORY TO AN INTERESTING SPECIAL SYSTEM

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The Positronium Hydride "molecule", composed of one atom each of positronium(Ps) and hydrogen (H), has one particle-stable state of total energy E = -1.575 Ry. In addition, it has an infinite Rydberg series of excited states, all of which are unstable against dissociation into Ps and H. Several calculational techniques will be discussed in connection with the evaluation of resonant and non-resonant scattering parameters for this unusual system. These will include the stabilization and complex-rotation methods as well as some less formal techniques.

1 Introduction

In this paper I will use the interesting special system called Positronium Hydride by chemists to illustrate certain calculational techniques. That is my primary purpose, but at the same time I must remark on the attractiveness of this system as a theoretical model with some possibilities (although distant) of experimental observation.

In fact, it was because of an observation made in the solid state that one of the earliest calculations of the binding energy of PsH was made by Neamtan et al [21]. The angular correlation between the gamma-rays due to positron annihilation in alkali hydride crystals had been measured [27] and was not then understood. This angular correlation measures the distribution in momentum of the positron-electron pair at the instant of annihilation. Neamtan et al [21] made the hypothesis that annihilation proceeded from a bound state of the positron with the hydride ion (H^-) inside the crystal. They used a simple trial function to represent the correlated PsH molecule and computed from it the angular correlation; it did not agree with experiment! I am not really interested in PsH in solids, where it is certainly perturbed from its free-space form, but such considerations still

motivate some work [2].

The PsH system consists of a proton (assumed fixed at the origin of coordinates), two electrons (r_1,r_2) and one positron (x). Its Hamiltonian, in Rydberg atomic units, takes the form

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_x^2 + 2[x^{-1} - r_1^{-1} - r_2^{-1} + r_{12}^{-1} - \rho_1^{-1} - \rho_2^{-1}], \quad (1.1)$$

where $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$, $\vec{\rho}_i = \vec{x} - \vec{r}_i$. To a large extent the complications in this kind of calculation arise from exchange combined with the need to use the positronium center of mass coordinate $\vec{R}_i = \frac{1}{2}(\vec{x}+\vec{r}_i)$ in order to satisfy the scattering boundary conditions.

To make things specific, let us examine the most important features of the PsH energy level diagram for both singlet and triplet electron-spin states. In Fig. 1 I show the particle-stable S=0 ground state at E ≈ -1.575 Ry [14], the Ps+H elastic scattering threshold at E = -1.5 Ry and a (PsH)* singlet resonance at E = -1.2 Ry, all of which will be discussed later on. Other interesting features include, positronium excitation thresholds, and the e^+-H^- and P_s^--H^+ thresholds at E = -1.05550203 Ry [10] and E = -0.524 Ry, respectively. In the rest of this paper I will discuss calculations of the bound state (including binding energy and annihilation rate), the singlet and triplet s-wave elastic scattering parameters (including the type of experiment most likely to succeed), and the position and width of the resonance shown. These are all based on techniques using only normalizable wave functions. Then, after a qualitative description of the

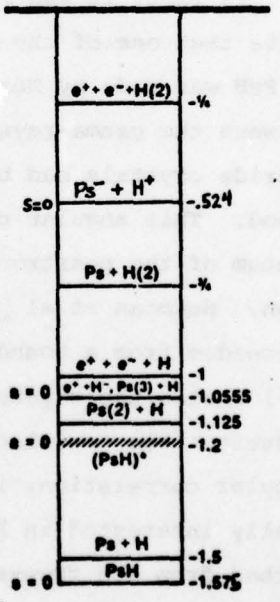

Fig. 1. Levels of PsH.

structure of the resonant state, I will outline an optical-potential calculation in progress, that should be applicable to some of the higher, narrower resonances occurring in all partial waves.

2 Rayleigh-Ritz and Stablization Calculations

The particle-stable ground state of PsH was discussed originally by Wheeler [29] and first shown to be bound in a variational calculation by Ore [22]. In the twenty-five years since then a series of variational energy determinations has been carried out with increasingly sophisticated trial functions, and the best present value of the binding energy [14] is slightly over 1 eV. Some idea of this progression is given in Table 1.

Table 1. History of PsH Binding Energy Calculations

DATE	REFERENCE	BINDING (eV)	TRIAL FUNCTION
1951	Ore [22]	0.0683	$\exp[-k(r_1 + \alpha r_2 + \beta\rho_2)] + 1\rightleftarrows 2$
1962	Neamtan et al [21]	0.228	$\exp[-(\alpha r_1+\beta r_2+\gamma\rho_1+\delta\rho_2)]+ 1\rightleftarrows 2$
1969	Lebeda & Schrader [19]	0.659	$* \Sigma\, C r_{12}^{m}(r_1^{i}r_2^{j}\rho_i^{k}\rho_2^{l}+1\rightleftarrows 2)$ (12 terms)
1973	Houston & Drachman[15]	0.6725	$e^{-\alpha x}[e^{-(z_1r_1 + z_2r_2)}+ 1\rightleftarrows 2]$ $*\Sigma\, C x^{l}[e^{-\beta r_1}r_1^{m}\rho_1^{n} + 1\rightleftarrows 2]$ (56 terms)
1974	Navin et al [20]	0.7946	(1969) * x (17 terms)
1974	Page & Fraser [23]	1.001	$e^{-\gamma x}\Sigma\, C x^{m} r_{12}^{k}[e^{-(\alpha r_1+\beta r_2)}r_1^{l}\rho_1^{n}$ $+ (1\rightleftarrows 2)]$ (70 terms)
1978	Ho [14]	1.0211	Same (210 terms)

While calculating the energy and some other properties of the PsH ground state using the Hylleraas type of trial function shown in Table 1, Houston and I observed [16] that one of the higher eigenvalues seemed to be "stabilized" [13]. This behavior

is shown in Fig. 2, which is taken from a later paper [7]. In this figure you see the convergence of the ten lowest eigenvalues of the truncated PsH hamiltonian as the expansion length, N, in-

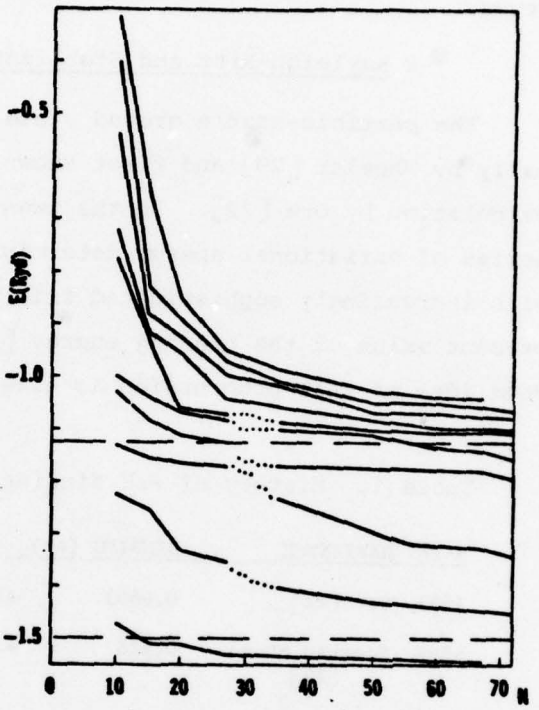

Fig. 2. First Ten Eigenvalues of the PsH Hamiltonian in Matrix Representation [7].

creases. The lowest eigenvalue descends below the elastic Ps-H threshold at N=13 and represents the bound state discussed above. Then there are some rapidly decreasing eigenvalues representing, in some sense, the elastic continuum and finally a very slowly decreasing or stabilized eigenvalue appears and indicates the existence of a resonance. The avoided crossing near N=30 is an important feature of the stabilization process; at this point the fourth eigenvalue replaces the third as the stabilized one. Another avoided crossing seems to occur just below N=70, but we were not able to pursue it further because of a loss in numerical accuracy in this region. We took the midpoint of this sloping

plateau as the position of the resonance, and the ¼ and 3/4 points to define the half-width, obtaining the resonance parameters $E_R = -1.1727$ Ry and $\Gamma = 5 \times 10^{-3}$ Ry. (These values should be taken as rough approximations only.) At the time we first reported this resonance [16] we noticed that it lay about 0.6 eV below the threshold for excitation of the 2s and 2p levels of positronium [Fig. 1], and we speculated idly on how this threshold could support such a resonance: The analogy with electron resonances below the n=2 threshold in hydrogen is not very close, since the present case involves two neutral sub-systems, and gives resonances only in singlet spin states. I will return to this question in Section 5.

3 Complex Rotation Method

It is certainly unnecessary to discuss, in this volume, the basic ideas involved in locating resonances by the complex-rotation or dilatation method [3,5,26]. Let me just remind you that one makes the substitutions $\vec{r}_i \to e^{i\theta} \vec{r}_i$ and $\vec{x} \to e^{i\theta} \vec{x}$ in the hamiltonian of Eq. (1.1), and numerically approximates the eigenvalues of the resulting non-Hermitian transformed hamiltonian

$$H(\theta) = e^{-2i\theta} T + e^{-i\theta} V, \tag{3.1}$$

where T and V are the kinetic and potential energy operators. Again we used a trial function like that in Table 1:

$$\Psi = e^{-(\alpha x + \beta r_1 + \gamma r_2)} \sum C(\theta)_{\ell m n} x^{\ell} r_1^m \rho_1^n + (1 \rightleftarrows 2) \tag{3.2}$$

to diagonalize H(θ) approximately. (Note that the expansion coefficients C will now be complex). In Figure 3 we show the appearance of the complex energy plane for θ=0.05, with the PsH bound state on the real axis, rotated cuts representing scattering outlined by discrete complex eigenvalues and a single, isolated resonant eigenvalue. You can see that the ideal behavior is not quite achieved by this numerical work; many eigenvalues lie near,

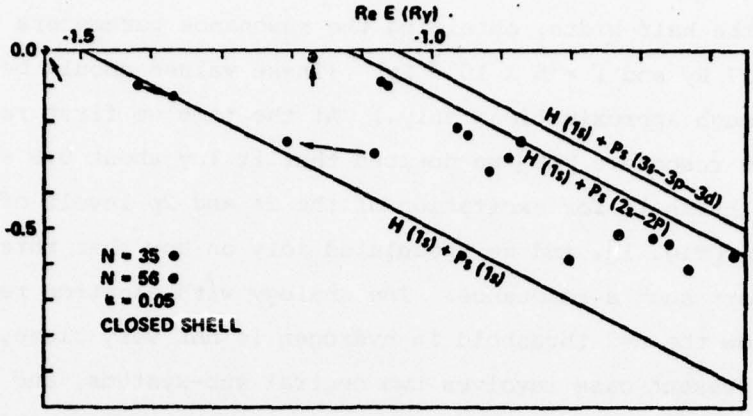

Fig. 3. Spectrum of the PsH Hamiltonian in matrix representation after dilation $r \to re^{i\theta}$.

but not on, the proper rays. So it is not surprising that the resonant eigenvalue when looked at more closely also is somewhat ambiguous. In Figure 4 such a closeup is displayed.

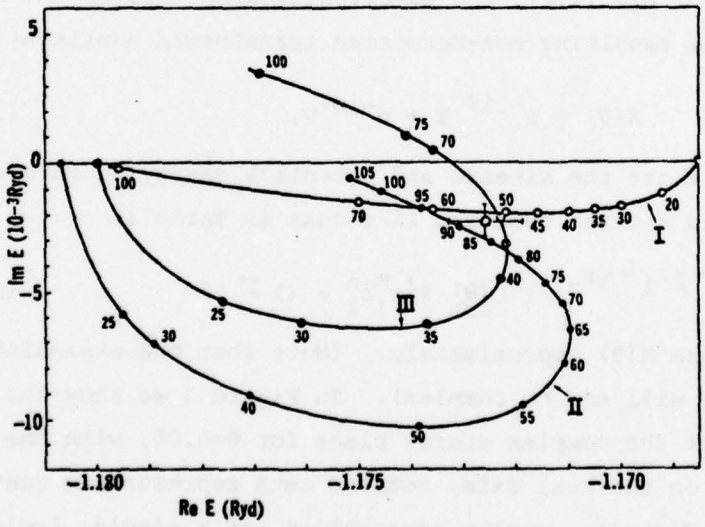

Fig. 4. Trajectories of the Resonant Eigenvalue for several sets of non-linear parameters [7].

We followed the empirical procedure recommended by Doolen [6]. For various sets of non-linear parameters (α,β,r), Figure 4 shows the paths traced out by the resonant eigenvalues as θ increases from 0 to 100 milliradians. These paths approach one another in a certain region and then diverge again; we consider this common region to approximate the complex energy $E_R - i\Gamma/2$ to which the rigorous theories refer. Some average of the various trajectory crossings is taken as the best result of the computation:

$$\begin{aligned} E_R &= -1.1726 \pm .0007 \text{ Ry} \\ \Gamma &= (4.6 \pm 1.1) \times 10^{-3} \text{ Ry} \end{aligned} \qquad [7] \qquad (3.3)$$

These results are seen to be very close to those obtained by the stabilization method. A very recent calculation, by the same technique, was performed by Ho [14]. As in the case of the ground state which I discussed in Section 2, Ho included the r_{12} correlation terms which Houston and I omitted. He found:

$$\begin{aligned} E_R &= -1.205 \pm .001 \text{ Ry} \\ \Gamma &= (5.5 \pm 2.0) \times 10^{-3} \text{ Ry}, \end{aligned} \qquad [14] \qquad (3.4)$$

where his E_R is much lower than ours and his Γ is consistent with ours; I will come back to this point in Section 5. Using a limited type of trial function in a Kohn variational calculation, Page [25] has found the parameters of this resonance to be

$$\begin{aligned} E_R &= -1.1738 \text{ Ry} \\ \Gamma &= 3.5 \times 10^{-3} \text{ Ry}, \end{aligned} \qquad [25] \qquad (3.5)$$

again not too far from our result.

You can see from Figure 4 (and from the similar diagram in [14]) that accurately locating the resonance position is difficult and ambiguous. Part of the trouble seems to stem from the fact that the trial function (3.2) was not chosen to emphasize any particular features of the PsH system. In particular, although we know that Ψ must be complex, we have used real basis functions and have put the burden on $C_{\ell mn}(\theta)$ to correct for this. Junker

[17] has suggested a choice of basis functions designed to represent better the various parts of the true resonant wave function, and perhaps his method should be applied here.

In a recent interesting paper [30] a criterion is given for selecting the best value of the resonance parameters in a case like that of Figure 4. It was shown there that, just as in the familiar case of a true bound state, the virial theorem should hold for the resonant eigenvalue, for any θ greater than the value first "uncovering" that eigenvalue. That is,

$$< T(\theta)> = - \frac{1}{2} < V(\theta)>, \qquad (3.6)$$

where T and V are complex. One can select the best value of the complex resonant energy by choosing θ to satisfy (3.6) as closely as possible. I am now re-examining some of our old results with this idea in mind.

4 Non-Resonant Scattering

Let me digress from the hunt for resonances which is the main theme of this article, to examine the non-resonant elastic scattering of positronium by hydrogen. This problem was treated in the exchange approximation by Fraser [11] and more exactly by Hara and Fraser [12]. Since they examined both electron-spin singlet(+) and triplet(-) states, they could calculate both total and Ps ortho-para conversion cross-sections. (Curiously enough, the latter is the first Ps-H process to be experimentally investigated [18], but so far only an upper limit has been obtained.) Using an effective-range expansion one can, extrapolate their singlet scattering results to estimate the PsH binding energy B in the exchange approximation:

$$\sqrt{2B} \cong \frac{1}{a} + r_o B. \qquad (4.1)$$

Here the scattering length and effective range have the values (in Bohr radii)

$$a^{(+)} = 7.275,\ r_o^{(+)} = 3.06 \qquad [\text{exchange}] \qquad (4.2)$$
$$a^{(-)} = 2.476,\ r_o^{(-)} = 1.44$$

Equation (4.1) leads to a value for the binding energy of B = 0.0193 Ry = 0.263 eV. Although this result is slightly better than the 1962 variational value [21], it falls far short of the more recent results; the implication is that adding correlation to the scattering calculation should improve the results considerably.

A straightforward technique to use one of the correlation functions of Table 1 in a scattering calculation is the Kohn variational method. In fact, Page [24] has carried out such a calculation for zero energy using a correlation function like that of [15] and including 35 terms. His results are

$$a^{(+)} = 5.844,\ r_o^{(+)} = 2.90 \qquad [\text{Kohn}] \qquad (4.3)$$
$$a^{(-)} = 2.319$$

(The effective range $r_o^{(+)}$ is obtained from Eq. (4.1) using the value of B of [23]; this is slightly inconsistent but $r_o^{(+)}$ is rather insensitive. No value of $r_o^{(-)}$ was presented since no triplet bound state exists.) These scattering lengths are rigorous upper bounds on the true values.

Let me describe the simple method used by Houston and me [7,8] to extract scattering information directly from the functions used previously [Eq. (3.2)]. The method is based on suggestions of Temkin [28] and Hazi & Taylor [13]. The idea is that a normalizable function whose energy expectation value lies in the continuum must approximate the scattering function of the same energy. [I am referring, for example, to the eigenfunctions corresponding to those non-stabilized eigenvalues in Figure 2 which lie in the range $-1.5 < E < -1.125$]. Inside the range of the scattering potential these wave functions may be very good, while asymptotically they fail completely, decaying exponentially rather than oscillating. Between these two regions there may be a sizable

intermediate region where the function displays scattering behavior before the inevitable decay sets in.

For the present case, we focus attention on the positronium center of mass wave function by projecting onto the ground states of Ps and H:

$$F(R_1) = \int\int \vec{d\rho}_1 \vec{dr}_2 \varphi_{Ps}(\rho_1)\psi_H(r_2)\Psi_E(\vec{r_1},\vec{r_2},\vec{x}), \tag{4.4}$$

where φ, ψ are the ground eigenstates of the positronium and hydrogen hamiltonians of Eq. (1.2). Ψ_E is a function of the form of (3.2) corresponding to a non-resonant energy E (for triplet scattering the sign of the exchange term in (3.2) is negative.) The "asymptotic" form should be

$$F(R) = \frac{A \sin(kR+\eta)}{R}, \tag{4.5}$$

where $k = (2E+3)^{\frac{1}{2}}$. The integral in (4.4) was evaluated numerically for a number of values of R, and for every pair of such values A and η were determined. In Figure 5 we show a plot of A and η (for the triplet case) as an example. Over the range $4 \le R \le 6$ both A and η are constant, and we interpret this as the appropriate intermediate "asymptotic" region in which to determine the phase shift.

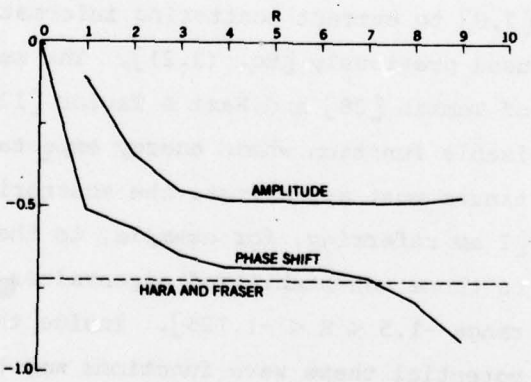

Fig. 5. Illustration of the method used to extract phase shifts from center-of-mass functions: the best s=1 case [8].

Since we do not have full control over the energies E, it is convenient to make an effective range fit to the points available. In Figure 6 I show the effective range function, k ctn η, plotted against the center of mass energy, $k^2/2$, for both triplet and singlet scattering. For the triplet case, a linear least-squares fit is very good; for the singlet case a more complicated fit including information about the bound state (4.1) is needed.

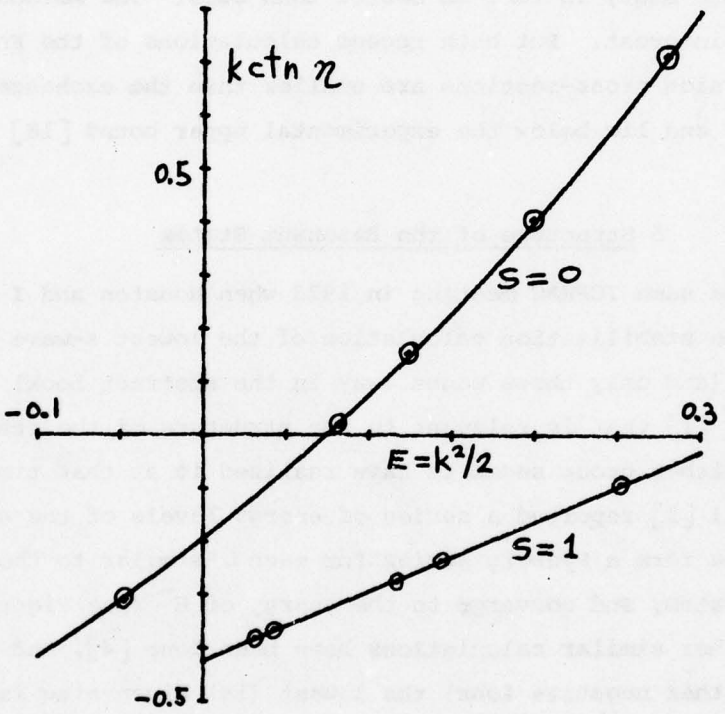

Fig. 6. Effective-range plots for S=0 and s=1. Circles contain the calculated values.

In this way the following scattering parameters can be derived:

$$a^{(+)} = 5.14 \qquad r_o^{(+)} = 2.44$$
$$a^{(-)} = 2.36 \qquad r_o^{(-)} = 1.31 \tag{4.6}$$

(These singlet parameters differ somewhat from those of Ref. [7]

where a different interpolation was used.) The zero-energy cross-sections are then [11].

$$\sigma \text{ (total)} = (a^{(+)^2} + 3a^{(-)^2}) = 43.1\ \pi a_o^2$$
$$\sigma \text{ (conversion)} = \tfrac{1}{4}\,(a^{(+)} - a^{(-)})^2 = 1.9\ \pi a_o^2. \qquad (4.7)$$

Since no bound principle holds for this kind of calculation we do not claim that our results are better than those of Page [24]; his triplet value must, in fact be better than ours. The method itself is of interest. But both recent calculations of the Ps ortho-para conversion cross-sections are smaller than the exchange value [12], and lie below the experimental upper bound [18] of $18\pi a_o^2$.

5 Structure of the Resonant States

At the same ICPEAC meeting in 1973 when Houston and I first reported the stabilization calculation of the lowest s-wave resonance [16] (and only three pages away in the abstract book) there was a paper [1] that is relevant to the structure of the resonance, although neither group seems to have realized it at that time. Arifov et al [1] reported a series of energy levels of the system e^+H^-. These form a Rydberg series for each L similar to those of a hydrogen atom, and converge to the energy of H^- (see Figure 1). Recently other similar calculations have been done [4], and for H^- (and most other negative ions) the lowest (1s) eigenvalue is not deep enough to produce a system stable against breakup into Ps + H as we know must be the case. But, at the same time, the 2s state lies very close to the resonance position! It should not have been difficult to conclude that the reported resonance [16] was mainly due to the e^+H^- component and its width was due to coupling with the open Ps-H channel, especially when one notes the absence of resonances for the triplet case [8].

Further support for this picture was provided by Ho [14]. He examined the effect on the resonance of removing certain types of correlation terms from his 210-term wave function: First, when he removed the inter-electronic coordinate r_{12} the energy rose by 0.032 Ry while the width did not change (Eqs. 3.3 and 3.4). He noted that this energy shift is very close to the correlation energy of H^- itself; by omitting r_{12} one seems to raise the energy of H^- along with the e^+H^- resonant state. Second, when he removed ρ terms only, the energy was unaffected, indicating that the central potential alone determines the binding energy of e^+ to H^- (the frozen-core approximation); no width calculation could be done since the breakup channel involves positronium with its ρ coordinate. From these facts we may conclude that a wave function of the following type should describe the s=0 resonant scattering well:

$$\Psi = \sum_n [F_n(R_1)\varphi_{Ps}^n(\rho_1)\Psi_H^{1s}(r_2) + (1 \leftrightarrows 2)] + \sum_m C_m G_m(x) \cdot \Phi_{H^-}(r_1 r_2). \quad (5.1)$$

(Clearly, since H^- exists for S=0 only, no such resonance occurs for S=1). Here we have summed over n, the quantum numbers of the open positronium channels (in practice only 1s, 2s, 2p) and have summed over the resonant terms labeled by m.

If we use this scattering trial function in a Kohn variational principle in the usual way and vary F_n and C_m, we obtain the coupled optical-potential equations:

$$\sum_{n'} L_{nn'}F_{n'}(R) + \sum_{n'm} \frac{1}{E-\epsilon_m} V_{nm}(R) \int d\vec{R}' V_{n'm}(R')F_{n'}(R) = 0. \quad (5.2)$$

The positron functions G_m and energies ϵ_m come from solution of the one-particle frozen-core equation:

$$\epsilon_m = \langle \Phi(12)G_m(x)H\,G_m(x)\Phi(12) \rangle, \quad (5.3)$$

$$\int dx\, G_m(x)\, G_{m'}(x) = 0 \quad (5.4)$$

The other quantities in Eq. (5.2) are defined as follows:

$$L_{nn'}F_{n'}(R_1) = \iint d\vec{\rho}_1 d\vec{r}_2 \varphi^n(\rho_1)\Psi(r_2)[H-E] \cdot[F_{n'}(R_1)\varphi^{n'}(\rho_1)\Psi(r_2) + (1 \rightleftarrows 2) \tag{5.5}$$

$$V_{nm}(R_1) = \iint d\vec{\rho}_1 d\vec{r}_2 \varphi^n(\rho_1)\Psi(r_2)[H-E]\, G_m(x)\Phi(12). \tag{5.6}$$

(These equations are exactly those of the Feshbach method [9], except that E does not vanish in Eq. (5.6) since no projection or orthogonalization was done.). In the single-channel case, below the inelastic threshold at Ps energy of $\frac{3}{8}$ Ry or 5.1 eV, the equation is:

$$-\tfrac{1}{2}[\nabla_R^2 + k^2]\, F(R) + \int d\vec{R}'\ K(R,R')\, F(R') + \sum_m \frac{V_m(R) \int d\vec{R}'\ V_m(R')\, F(R')}{E - \epsilon_m} = 0 \tag{5.7}$$

(Here the direct potential vanishes by symmetry, K is the kernel given in [11] and one must remember that V_m is energy dependent.) This equation is presently under study, and should give reasonable values for resonance positions and widths.

6 Conclusions

I have described the PsH system - its spectrum of bound and low-lying resonant states and its elastic scattering parameters - for the purpose of illustrating physical and computational ideas. These include variational, stabilization, complex-rotation and optical potential methods of calculation, and the physical description of systems deduced from the behavior of wave functions. I hope I have conveyed a feeling for the interaction between physical insight and computation that is, I believe, one of the most satisfying aspects of theoretical physics.

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DISCRETIZATION, QUADRATURES, AND BASIS SETS FOR THE TWO-ELECTRON EJECTION PROBLEM

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Results from earlier work on discretized spectra of one-body scattering Hamiltonians are reviewed, and a rough and ready "quadrature" approach to the cross section $h\omega + H^- \rightarrow H + e^- + e^-$ discussed. The challenge of the Wannier threshold is discussed in terms of new classifications of two-electron states developed by Wulfman and Herrick.

1 Introduction

The problem of representation of the resolvent of an operator with a continuous spectrum by discretization in a finite basis of L^2 functions has a long history: in particular it is the root of the "spurious" singularities in the Kohn method as discussed by Schwartz.[1] However, understanding the relationship of the discretized spectrum to the actual spectrum of the operator not only leads to removal of the Kohn singularities, but gives rise to a family of discrete methods in quantum scattering theory which have proven to be highly effective computational methods in their own right. In Sections 2 and 3 we discuss finite and infinite dimensional discretizations, the former yielding Gauss quadrature representations, the latter "distributions" equivalent to the actual "continuum" scattering eigenfunctions.

In Section 4 a combination of the two techniques is applied to calculation of the double detachment cross section

$$\hbar\omega + H^- \rightarrow H^+ + e^- + e^-$$

and is found wanting in several respects. Possible remedies are discussed in Section 5.

2 L^2 Discretization-Finite Quadratures

Suppose we have a one-body radial Hamiltonian, $H = p^2/2m + V(r)$, such as might arise in the theory of potential scattering.

Diagonalization of the matrix representation $\bar{H}$, taken with respect to a finite subset of a complete, discrete set of functions, yields L^2-normed, orthogonal matrix eigenfunctions $\bar{\chi}_i$:

$$\bar{H}\bar{\chi}_i = \varepsilon_i \bar{\chi}_i, \tag{2.1a}$$

$$\langle \bar{\chi}_i, \bar{\chi}_j \rangle = \delta_{ij}. \tag{2.1b}$$

We can now inquire as to the relationship between those $\bar{\chi}_i$ whose corresponding matrix eigenvalues occur at positive energies (i.e., at energies where H itself has a continuous spectrum) and the actual "eigenfunctions" of H which are δ-function normed:

$$H\chi_E = E\chi_E \quad (E>0) \tag{2.2a}$$

$$\langle \chi_E, \chi_{E'} \rangle = \delta(E-E'). \tag{2.2b}$$

Any attempt to equate the discretized spectral resolution

$$I = \sum_i |\bar{\chi}_i\rangle\langle\bar{\chi}_i| \tag{2.3a}$$

with the identity (neglecting bound states)

$$I = \int dE |\chi_E\rangle\langle\chi_E| \tag{2.3b}$$

can only succeed in a restricted range of coordinate space defined by the choice of finite basis. However, we might expect that for suitably localized functions f(r), g(r) that

$$\langle f,g \rangle = \int dE \langle f|\chi_E\rangle\langle\chi_E|g\rangle \approx \sum_i \langle f|\bar{\chi}_i\rangle\langle\bar{\chi}_i|g\rangle \tag{2.4}$$

to any desired practical accuracy, thus allowing the use of the spectral theorem for calculation of <u>moments</u> with respect to localized functions.

The precise relationship between the spectral resolutions of Eq. (2.3a) and (2.3b) has been worked out for the radial kinetic energy, and radical attractive and repulsive Coulomb problems.[2,3] The result is that Eq. (2.3a) is a Gaussian

quadrature approximation to Eq. (2.3b), valid in the above mentioned sense of moments. In particular, we can equate (again in the sense of moments)

$$|\bar{\chi}_i\rangle = \sqrt{\omega_i^{Eq}}\,|\chi_{E_i}\rangle \tag{2.5}$$

embodying the suggestion that in the region defined by the L^2 expansion basis that the essential difference between the unit-normal $|\bar{\chi}_i\rangle$ and the δ-function normed continuum eigenfunction $|\chi_{E_i}\rangle$, corresponding to the same energy, is effectively a normalization, which is in fact a Gaussian quadrature weight. More particularly diagonalization of the radial kinetic energy in a basis of the type

$$\phi_i^{Slater}(r) = r^{\ell+1}e^{-r/2}\,L_n^{2\ell+2}(r) \tag{2.6}$$

($L_n^{2\ell+2}(r)$ being a generalized Laguerre polynomial) leads to an ultraspherical polynomial quadrature, whereas a basis of the type

$$\phi_i^{Gaussian}(r) = e^{-r^2}\,H_n(r) \tag{2.7}$$

($H_n(r)$ being an Hermite polynomial) yields a Laguerre quadrature.

A more interesting quadrature arises in the Coulomb case[3] when discretization of the repulsive Coulomb problem

$$H_+^{Coul} = p^2/2m + \frac{1}{r} \tag{2.8a}$$

in the Laguerre set of Eq. (2.6) yield the (singular) Pollaczek quadrature which follows, in the theory of classical orthogonal functions, from use of a measure with an essential singularity at each end of the integration range. The attractive Coulomb problem

$$H_-^{Coul} = \frac{p^2}{2m} - \frac{1}{r} \tag{2.8b}$$

yields a modified Pollaczek quadrature which reproduces moments

of the spectral expansion over both bound and continuum states. It is amusing to note that the essential singularity in the measure function of Pollaczek may be identified with the Coulomb essential singularity corresponding to the accumulating bound states at E = 0.

As a specific example[3] of the efficiency of the quadrature representation for the Coulomb problem we have computed the hydrogen photo-effect cross section by direct diagonalization of Eq. (2.8b) in the basis of Eq. (2.6), and assuming

$$\sigma_{\text{photoionization}}(E) \equiv \left|\langle\phi_{1s}|d|\chi_E^{\text{Coul}}\rangle\right|^2 \cong \frac{\left|\langle\phi_{1s}|d|\bar{\chi}_i\rangle\right|^2}{\omega_i^{\text{Eq}}} \tag{2.9}$$

$\bar{\chi}_i$ being the discretized, unit normalized matrix eigenfunction, and ω_i^{Eq} the appropriate modified Pollaczek quadrature weight; ϕ_{1s} is the H atom ground state wavefunction and d the dipole operator.

As shown in the following table the L^2 discretization is capable of producing extraordinarily accurate results, given

Table 1 H atom photo effect cross sections calculated using a Laguerre-type discretization involving only L^2 functions. It is clear that the discretized spectrum provides an excellent representation of the actual final state Coulomb wavefunction.

Photon Energy (a.u.)	N = 10*	N = 15	Exact (a.u.)
0.51	0.21359	0.21354006	0.2135401
0.60	0.137834	0.13783051	0.13783050
0.70	0.090390	0.090392075	0.090392081

*N is the number of basis functions used to discretize both the bound state and continuous spectrum of atomic H. $\lambda = 1.5$ in these calculations which are those of Ref. 3.

that the representation $|\bar{\chi}_i\rangle/\omega_i^{Eq}$ of the actual Coulomb continuum function is only sampled by its overlap with the highly localized function $d|\phi_{1s}\rangle$.

Generalizations of these quadrature ideas are implicit in the moment-imaging work of Langhoff[4] and co-workers, and explicit in the work of Broad,[5] to be discussed in the following section.

3 L^2 Discretization-Infinite Basis

For the simple one-body Hamiltonians discussed in Section 2, where Laguerre discretization gives simple Gaussian quadrature interpretations of the spectra, it is also possible to analytically diagonalize the corresponding infinite dimensional problem.[6,7] This follows from the fact that use of the nonorthogonal basis

$$\phi_i(r) = r^{\ell+1} e^{-r/2} \quad L_n^{2\ell+1}(r) \tag{3.1}$$

tridiagonalizes both H and the overlap. The resulting infinite dimensional matrix representation of the Schrodinger equation

$$\bar{\bar{H}}\bar{c} = \lambda\bar{\bar{S}}\bar{c} \tag{3.2}$$

is thus equivalent to a three-term recursion scheme, which may be solved exactly via a related difference equation.[3,7]

For example the normal radial scattering function

$$\langle r|\Psi_E\rangle = \left(\frac{2}{k\pi}\right)^{1/2} (kr) j_\ell(kr), \tag{3.3a}$$

$j_\ell(kr)$ being the ℓ^{th} wave spherical Bessel function also has the representation

$$\langle r|\Psi_E\rangle \underset{D}{=} B_\ell(E) \sum_{n=0}^{\infty} \frac{n!}{\Gamma(n+2\ell+2)} C_n^{\ell+1}(x)\, \phi_n(r) \tag{3.3b}$$

where the ϕ_n are those of Eq. (3.1), $C_n^{\ell+1}(x)$ are ultraspherical polynomials in $x = (E-1/8)/(E+1/8)$, and $B_\ell(E)$ is the normalization

$$B_\ell(E) = \left(\frac{2}{\pi k}\right)^{1/2} 2^\ell(\ell!)(1-x^2)^{(\ell+1)/2}, \tag{3.3a}$$

th similar but more complex results for the attractive and repulsive Coulomb problems. The $\underset{D}{=}$ in Eq. (3.3b) indicates that the equality is to be understood in the sense of distributions.[9]

Th xistence of these exact infinite expansions in terms of L ions has given rise to the "J-matrix" or Jacobi techn for solution of the usual close coupling equations of atomic scattering theory, the name arising from the tridiagonal form of Eq. 3.2. Rudiments of such a theory appear in Refs. 6 and 7, and a discussion of the lack of "spurious" singularities appears in Ref. 8--the singularities disappear as the infinite matrix problem has a continuous spectrum. The theory has been completely developed for the general LS coupling atomic scattering case,[10] and applied to the photo effect in H^-, both to single and double detachment, discussed in the following section. Additionally Broad[5] has used the J-matrix formalism to extend the Gauss quadrature ideas of Section 2 to a wide class of interaction potentials.

4 Two-Electron Continuua

One clear mathematical and computational frontier is the problem of treatment of two (or more!) slowly moving unbound electrons in the presence of a third charged particle, which we assume to be infinitely massive. This situation arises in impact ionization,

$$e^- + A \to A^+ + e^- + e^- \tag{4.1}$$

or double detachment

$$\hbar\omega + A^- \to A^+ + e^- + e^-, \tag{4.2}$$

both producing the same three-body final state. Near threshold for either of these processes the outgoing electrons are strongly

correlated over large volumes of phase space giving rise to very strong angular momentum transfer[12] and the Wannier threshold[13] law

$$\sigma_{\text{ThreeBodyProduction}} \sim E^{1.127} \tag{4.3}$$

in contrast to the usual Wigner[14] threshold law. From a computational point of view the three-body final state gives rise to a continuum of open channels, and also, within the usual close coupling framework, an expansion in target angular momentum states which is unlikely to converge. This latter statement following from Fano's analysis of angular momentum transfer near threshold.[12]

The problem of the continuum of open channels can be attached using the quadrature ideas of the previous sections. Broad and Reinhardt[11] have calculated the cross section

$$\hbar\omega + H^- \rightarrow H^+ + e^- + e^- \tag{4.4}$$

using the Pollaczek discretization[3] of the bound and continuum target states implied by use of a Laguerre discretization. Cross sections are shown in Figures 1 and 2. The close coupling equations were solved using the J-matrix technique of Section 3. The "quadrature" nature of the pseudo-state discretization of the three-body final state is apparent from the noise in Figure 2; however, the cross section does seem to be converging a few eV above the three-body threshold. On the other hand the close-coupling expansion does not converge near threshold because of our inability to include enough target angular momentum states. How might a better "two-electron" expansion basis be chosen?

5 Two-Electron States: New Classifications

The problem of more natural choices of basis for strongly correlating two-electron systems has been approached by

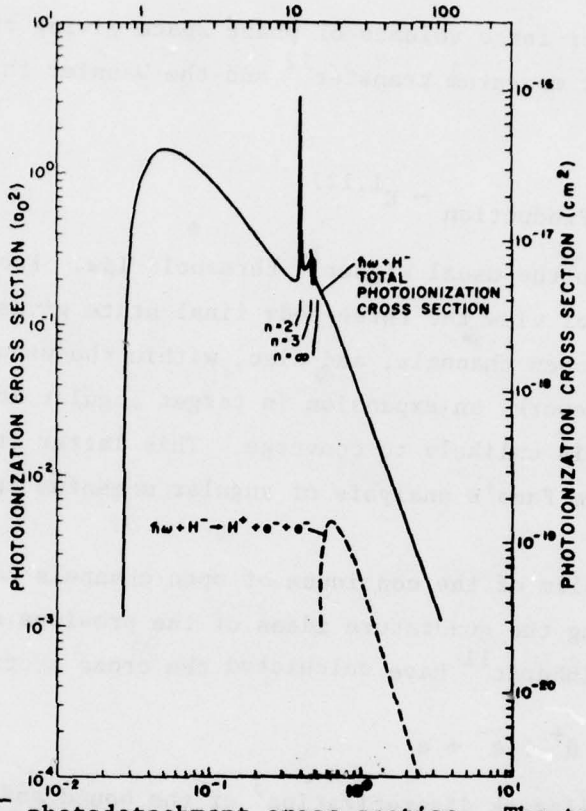

Figure 1. H^- photodetachment cross section. The total cross section and two-electron ejection cross sections are shown over a wide range of photon energies (in eV and a.u.).

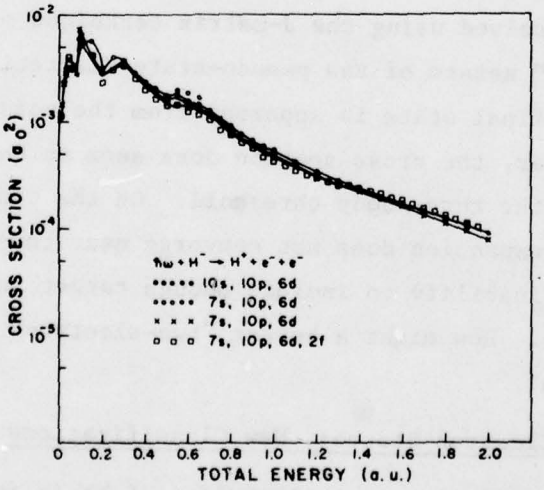

Figure 2. Pollaczek quadrature estimate for the double detachment of H^-. Convergence near threshold is poor, as the quadrature is of low order in that region.

Wulfman,[15] and by Herrick,[16,17] from a group theoretical point of view. We end our discussion by summarizing some of their simpler results, followed by speculation about extension into the break up region.

The new classification and construction of two-electron "correlated" states follows from the Runge-Lenz classification of one-electron states of the H-atom, introduced by Pauli[18] in 1926. The ideas are most easily visualized classically (or semi-classically in terms of "Bohr" orbits), where we note that the -1/R (Kepler) potential gives rise to elliptical orbits <u>which do not precess</u>. The vector from the center of force (i.e., the nucleus, with mass turned off) along the major axis of the planar ellipse is thus a constant of the motion, referred to as the Lenz, or Runge-Lenz vector, $\vec{A}$, with a corresponding quantum mechanical operator (for details see Refs. 15, 16 or the elementary discussion of Schiff, Ref. 18). In the usual L-S coupling scheme one works with two-electron configurations of the form $|n\ell,n'\ell',L,S>$, which diagonalize L^2, L_z, S^2, S_z, but certainly <u>not</u> the two-electron Hamiltonian. Wulfman[15] and Sinanoglu and Herrick[16a] noted that if one also diagonalizes $\vec{A}_1 - \vec{A}_2$, the difference between the Runge-Lenz vectors of the two electrons, one comes very close to having diagonalized $1/|r_1-r_2|$ itself, provided that $n = n'$, that is, provided that we are within a degenerate subshell. Herrick and Sinanoglu,[16b] have extended these ideas to intershell correlations, finding empirically the existence of new, and approximately "good" quantum numbers. It appears through these group theoretic and empirical studies that diagonalization of the operator equivalent, $\vec{A}_1 - \vec{A}_2$, (which may be done in closed form via appropriate group theoretic algebra) accounts for as much as 90 to 98% of inter- and intra-shell correlations between highly excited electrons. Apparently, what has been achieved is an angular momentum recoupling and mixing appropriate to two strongly correlated electrons. Herrick[19] has begun extensions

to classifications of continuum states, but the fact remains that these powerful techniques have been used neither in usual bound-bound excitation close-coupling calculations, or in approaches to the two-electron ejection threshold. It is in the realm of equivalent or nearly equivalent highly excited electronic states that one has the most to gain by working in such a correlated basis. I venture to conjecture that a successful computational approach to the Wannier problem involving these ideas will appear within the next several years.

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MATRIX VARIATIONAL CALCULATIONS OF ELECTRON-ATOM SCATTERING

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The continuum variational method of Kohn has been developed into a practical computational method in electron-atom scattering theory. This algebraic or matrix variational formalism is reviewed, with emphasis on the computational procedures necessary for applications to inelastic scattering processes. The matrix variational method has been used to obtain quantitative theoretical results relevant to recent experimental research. Examples of such applications will be given.

1 Introduction

A quantitative theory of electron-atom scattering, valid in the energy range below the first ionization threshold, must describe short-range correlation effects and also provide an accurate treatment of long-range scattering by multipole potentials. In the matrix variational method [1,2] both short-range and long-range components of the scattering wave function are expanded as linear combinations of specified basis functions. Variational theory is used to compute the coefficients. Computational procedures reduce to the manipulation of matrices of the Hamiltonian operator, represented in the given bound and continuum basis.

Several review articles have described the variational method [1,3,4,5], compared it with other methods valid for low-energy electron scattering [4] and surveyed results of calculations by these methods [5,6]. The present article is intended to review

the basic variational methodology, including some recent developments, and to survey briefly some interesting results obtained with this method.

2 Theory

Electron scattering by an N-electron atom is described by a Schrödinger wave function

$$\Psi = \Sigma_p \mathcal{A}\Theta_p\psi_p + \Sigma_\mu \Phi_\mu c_\mu \ . \qquad (1)$$

Here Θ_p is a normalized N-electron target state wave function, ψ_p is a one-electron channel orbital, antisymmetrized into Θ_p by the operator $\mathcal{A}$, and Φ_μ is an N+1-electron function constructed from quadratically integrable one-electron orbital basis functions. For nonrelativistic scattering by light atoms, Ψ can be taken to be an eigenfunction of $\underset{\sim}{L}^2$, $\underset{\sim}{S}^2$, and parity π, and the functions Θ_p and Φ_μ can be LS-eigenfunctions. $(\Theta_p|H|\Theta_q)$ is assumed to be diagonalized, with eigenvalues E_p, so that the channel orbital kinetic energy is

$$\frac{1}{2} k_p^2 = E - E_p \qquad (2)$$

in Hartree units, at total energy E. For closed channels ($k_p^2<0$), k_p is replaced by $i\kappa_p$ with $\kappa_p>0$. The orbital angular momentum of ψ_p is ℓ_p. Channel orbital functions are of the form

$$\psi_p = f_p(r)Y_{\ell m_\ell}(\theta,\phi)u_{m_s} , \qquad (3)$$

where $f_p(r)$ satisfies the usual boundary conditions at r=0. It is assumed that ψ_p is orthogonal (by construction) to all orbital functions used in constructing Θ_p and Φ_μ.

As $r\to\infty$ in each open channel, for multichannel scattering by a neutral atom,

$$f_p(r) \sim k_p^{-1/2} r^{-1} [\sin(k_p r - \tfrac{1}{2}\ell_p\pi)\alpha_{op} + \cos(k_p r - \tfrac{1}{2}\ell_p\pi)\alpha_{1p}] \ . \tag{4}$$

This functional form is modified for Coulomb or dipole scattering. Scattering matrices and cross sections are determined by the coefficients α_{ip}, i=0,1. Variational expansion of the quadratically integrable component of Ψ gives a system of inhomogeneous linear equations for the coefficients $\{c_\mu\}$ [7]. Formal solution of these equations reduces the variational functional

$$\Xi = (\Psi|H-E|\Psi) \tag{5}$$

to the quadratic expression [2,4]

$$\Xi = \Sigma_{ij}\Sigma_{pq}\alpha^*_{ip} m^{pq}_{ij} \alpha_{jq} \ . \tag{6}$$

Exact solution of the Schrödinger equation would require

$$\Sigma_j \Sigma_q m^{pq}_{ij} \alpha_{jqs} = 0 \ , \tag{7}$$

for N_C linearly independent degenerate solutions, indexed by s, where N_C is the number of open channels at given energy E.

In a matrix notation that suppresses open-channel indices and summations, Eq. (6) is

$$\Xi = \alpha^{\dagger} m \alpha \tag{8}$$

and Eq. (7) is

$$m\alpha = 0 \ . \tag{9}$$

The set of N_C solution vectors is the $2N_C \times N_C$ rectangular matrix

$$\alpha = \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} \tag{10}$$

where α_0 is the $N_C \times N_C$ array α_{0ps} and α_1 is the array α_{1ps}. Similarly, m_{ij}^{pq} is an element of the $2N_C \times 2N_C$ square matrix

$$m = \begin{bmatrix} m_{00} & m_{01} \\ m_{10} & m_{11} \end{bmatrix} . \tag{11}$$

All matrix elements are real, m_{00} and m_{11} are symmetric, but

$$m_{01} - m_{10}^{\dagger} = \frac{1}{2} I \ , \tag{12}$$

as a consequence of the asymptotic normalization of the channel orbitals. Here (†) denotes the transpose or Hermitian adjoint and I is a unit matrix.

A particular canonical form for α is

$$\alpha_0 = I, \qquad \alpha_1 = K \tag{13}$$

where K is the <u>reactance matrix</u> [8], real and symmetric for

exact solutions. For matrices α of general form, if α_0 is nonsingular,

$$K = \alpha_1 \alpha_0^{-1} . \tag{14}$$

Scattering matrices and cross sections are computed from K.

Solutions of the expected form require m to have N_c zero eigenvalues. Since this condition is not generally satisfied by approximate solutions, it is necessary to consider variational estimates of α.

An oscillatory function that does not vanish as $r \to \infty$ cannot be represented as a finite superposition of quadratically integrable functions. For this reason, the open-channel terms $\mathcal{A}\Theta_p\psi_p$ in Eq. (1) remain distinct from the bound or Hilbert space component $\Sigma_\mu \Phi_\mu c_\mu$. Closed-channel terms can be included in the form $\mathcal{A}\Theta_q\psi_q$ as in the usual close-coupling expansion [9], used also in R-matrix calculations [10]. Target atom polarization is represented by including an explicit polarization pseudostate function Θ_q as a closed-channel term [11,12]. An alternative approach, based on a hierarchy of continuum Bethe-Goldstone (BG) equations [13], represents target atom polarization and correlation effects by including suitable basis functions $\{\Phi_\mu\}$ in the bound component of Ψ [2,4]. Matrix variational

calculations for atoms other than hydrogen have used the BG formalism [4,6].

3 Variational Formalism

For an infinitesimal variation of α, the variation of the functional Ξ is

$$\delta\Xi = \delta\alpha^\dagger m\alpha + (m\alpha)^\dagger\delta\alpha + \frac{1}{2}\,(\alpha_0^\dagger\delta\alpha_1 - \alpha_1^\dagger\delta\alpha_0) \ , \tag{15}$$

using Eq. (12). In the multichannel Kohn method [14,15], α_0 and α_1 are defined as in Eqs. (13), so that

$$\delta\alpha_0 = 0, \qquad \delta\alpha_1 = \delta K \ . \tag{16}$$

Then

$$\delta\Xi = \delta K^\dagger(m_{10}+m_{11}K) + (m_{10}+m_{11}K)^\dagger\delta K + \frac{1}{2}\,\delta K \ . \tag{17}$$

If K_t is a trial matrix such that

$$m_{10} + m_{11}K_t = 0 \ , \tag{18}$$

then the Kohn functional

$$[K] = K_t - 2\Xi(K_t) = -2(m_{00} - m_{10}^\dagger m_{11}^{-1} m_{10}) \tag{19}$$

is stationary, and equals K_t when Ξ goes to zero, as for an exact scattering solution. The matrix [K] is real and symmetric. It has anomalous singularities at singular points of the matrix m_{11}. If $\alpha_0 = K^{-1}$ and $\alpha_1 = I$, a similar expression (inverse Kohn)

can be derived for $[K^{-1}]$, with anomalies at singular points of m_{00}. These anomalies can be avoided by alternative use of the Kohn and inverse Kohn methods [15], in the neighborhood of zero eigenvalues of m_{00} or m_{11}, respectively.

Each element of m has a pole at each eigenvalue of the bound-bound matrix $(H-E)_{\mu\nu}$. It has been shown [15] that these poles cancel exactly in Eq. (19) and do not cause spurious singularities in [K], contrary to the original interpretation of the anomalies found in variational calculations [7]. However, each element of m takes on all possible real values between successive poles. The submatrices m_{00} and m_{11} must each have a zero eigenvalue for some value of E between each pair of successive poles, although there is no reason in general for these singular points to coincide. This behavior is shown in published examples [3,5,15]. The resulting anomalies in [K] are computational artifacts, since the number of singularities is governed by the number of basis functions Φ_μ included in Eq. (1).

If these anomalies occurred at eigenvalues of the bound-bound matrix, as originally assumed, they could be avoided only by varying parameters in the bound basis functions, so as to displace these eigenvalues. However, since the anomalies in [K] actually occur at singular points of m_{11}, they can be avoided

much more easily by using $[K^{-1}]$ near such points. The anomaly-free (AF) method [15] uses the ratio of determinants $|m_{00}|/|m_{11}|$ as a criterion for choice between [K] and $[K^{-1}]$.

This approach is not completely satisfactory, because results vary discontinuously except in the limit of exact solution. In energy ranges where rapidly varying physical scattering structures occur this is a serious difficulty.

In more sophisticated methods, a preliminary orthogonal transformation is carried out in the $2N_c$-dimensional linear space of the asymptotic open-channel wave functions [16]. The transformation matrix is

$$u = (\alpha\beta) \tag{20}$$

were α and β are both $2N_c \times N_c$ matrices, each consisting of N_c column vectors. The orthonormality conditions are

$$\alpha^\dagger\alpha = \beta^\dagger\beta = I; \qquad \alpha^\dagger\beta = \beta^\dagger\alpha = 0 \; . \tag{21}$$

The transformed matrix is

$$m' = u^\dagger m u = \begin{bmatrix} m'_{00} & m'_{01} \\ m'_{10} & m'_{11} \end{bmatrix} \tag{22}$$

$$= \begin{bmatrix} \alpha^\dagger m\alpha & \alpha^\dagger m\beta \\ \beta^\dagger m\alpha & \beta^\dagger m\beta \end{bmatrix} . \tag{23}$$

Any transformation u defines a trial matrix α_t. The problem is

to define a stationary matrix $[\alpha]$ that equals α_t for an exact scattering solution.

The K-matrix defined by Eq. (14) is not affected by any nonsingular linear transformation that does not mix column vectors of α and β. Hence the most general optimizing transformation is of the form [17]

$$[\alpha] = \alpha + \beta K' \tag{24}$$

where α and β are fixed and only K' varies. For an infinitesimal variation $\delta K'$,

$$\delta \Xi = \delta K'^{\dagger}\left(m'_{10}+m'_{11}K'\right) + \left(m'^{\dagger}_{10}+K'^{\dagger}m'_{11}\right)\delta K' + \left(m'_{01}-m'^{\dagger}_{10}\right)\delta K' \ , \tag{25}$$

similar to Eq. (17) except that Eq. (12) does not necessarily hold for m'. The matrices m'_{ij} defined by Eq. (22) are constant with respect to variations of K'. If m'_{11} is symmetric and

$$K'_t = -\left(m'_{11}\right)^{-1} m'_{10} \tag{26}$$

then

$$[K'] = -\left(m'_{01}-m'^{\dagger}_{10}\right)^{-1}\left[m'_{00}-m'^{\dagger}_{10}(m'_{11})^{-1}m'_{10}\right] \tag{27}$$

is stationary, and equals K'_t for an exact scattering solution. From Eq. (14), the reactance matrix is

$$K = (\alpha_1+\beta_1[K'])(\alpha_0+\beta_0[K'])^{-1} \ . \tag{28}$$

In the minimum-norm (MN) method [16], α is constructed from the eigenvectors of the positive definite matrix $m^{\dagger}m$ corresponding to its N_c lowest eigenvalues. [K'] is defined by Eq. (27) in the optimized version of this method (OMN) [17]. Because m'_{11} can be singular, anomalies still occur in this method.

Anomalies in Eq. (27) can be avoided by two alternative strategies, either to make m'_{10} vanish, or to ensure that m'_{11} is nonsingular. The first of these alternatives is implemented in the optimized anomaly-free (OAF) method [17,18]. The real unsymmetric matrix m is converted to upper triangular form by an orthogonal transformation unless it has complex eigenvalues. Since m'_{10} vanishes, Eq. (27) for the OAF method reduces to

$$[K'] = -(m'_{01})^{-1} m'_{00} \ . \tag{29}$$

Diagonal elements are permuted, while maintaining $m'_{10}=0$ and ensuring that m'_{01} is nonsingular, so that the minimal elements occur in m'_{00}. This is necessary for consistency, since m'_{00} as given by Eq. (23) is identical with the variational functional Ξ, which should vanish in the limit of an exact solution.

The OAF method does not in general make K symmetric, and results can be discontinuous when diagonal elements of m' of opposite sign cross in magnitude. Special provision has to be

made for complex eigenvalues of m [17,18]. Despite these difficulties, this method systematically avoids anomalies, and is less arbitrary than the AF method. The OAF method has been used for most of the variational results recently obtained.

A method that avoids anomalies, maintains the symmetry of the K-matrix, and produces continuous results has only recently been formulated [18]. If Eq. (12) holds for the transformed matrix m', then [K'], given by Eq. (27), is obviously symmetric, and it can be shown that these two conditions imply the symmetry of K. Orthogonal transformation matrices that preserve Eq. (12) have been shown to have the canonical form [18].

$$u = \begin{bmatrix} CX & -SX \\ SX & CX \end{bmatrix} = \begin{bmatrix} \alpha_0 & \beta_0 \\ \alpha_1 & \beta_1 \end{bmatrix} , \tag{30}$$

where X is orthogonal, and C and S are commuting real symmetric matrices such that

$$C^2 + S^2 = I . \tag{31}$$

Since X is irrelevant to the K-matrix, as given by Eq. (14), preliminary transformations of m can be restricted to the physically relevant class defined by

$$\alpha_0 = C, \qquad \alpha_1 = S , \tag{32}$$

with the properties given above.

The proposed "interpolated anomaly-free" (IAF) method [18] uses the second alternative strategy mentioned above, avoiding singularities by ensuring that m'_{11} is nonsingular. This is done by maximizing the magnitude of det m'_{11} for transformations of the physically relevant class, defined by Eqs. (32). Since no direct algorithm is known for constructing u to satisfy these conditions, an iterative procedure is required. It is found, however, that restricting C and S to be diagonal matrices produces satisfactory results, so more general transformations are probably not necessary. This restricted IAF method (RIAF) obtains C and S in the form

$$C_{pq} = \delta_{pq}\cos\phi_p ; \qquad S_{pq} = \delta_{pq}\sin\phi_p , \tag{33}$$

where the phase angles ϕ_p are chosen to maximize $|\det m'_{11}|$. The Kohn method corresponds to taking all ϕ_p=0, while for the inverse Kohn method all ϕ_p=$\pi/2$. Model calculations [18] show that this method is as accurate as the OAF method, but avoids the difficulties of the latter.

4 Implementation

Details of implementation have been given elsewhere [2,19]. The principal computational effort is calculation of the matrix m [15,19],

$$m_{ij}^{pq} = M_{ij}^{pq} - \Sigma_\mu \Sigma_\nu M_{ip,\mu}(M^{-1})_{\mu\nu}M_{\nu,jq} . \tag{34}$$

The matrices combined here are the bound-bound matrix

$$M_{\mu\nu} = (\Phi_\mu|H-E|\Phi_\nu) \ , \tag{35}$$

the bound-free matrix

$$M_{\mu,ip} = (\Phi_\mu|H-E|\mathcal{A}\Theta_p\psi_{ip}) \ , \tag{36}$$

and the free-free matrix

$$M_{ij}^{pq} = (\mathcal{A}\Theta_p\psi_{ip}|H-E|\mathcal{A}\Theta_q\psi_{jq}) \ . \tag{37}$$

Each of these matrix elements is a linear combination of definite integrals over the bound and free (continuum) radial basis function. Computational and data-handling algorithms for their calculation have been published [19].

The basic integrals involving continuum radial functions must be evaluated rapidly and accurately. Adequate analysis of alternative methods for the required two-electron integrals has been carried out [20] only for continuum functions in the form of spherical Bessel functions. This limits applications at present to scattering by neutral atoms. Formulas are available for Coulomb wave functions [21,22], but have not yet been tested sufficiently for general applications.

The dimension of the bound basis $\{\Phi_\mu\}$ may be very large. Comparable bound state calculations can require several thousand

electronic configurations. The dimension of the free basis is much smaller, essentially $2N_c$, for N_c open channels. Since $M_{\mu\nu}$ can be very large, the direct computation of its inverse, apparently required in Eq. (34), would be very inefficient. This task is made tractable by an algorithm [23] that adapts the well-known Cholesky decomposition to the real symmetric but not positive definite matrix $M_{\mu\nu}$. This makes it possible to evaluate the second term in Eq. (34) in terms of a matrix product $T^{-1}M$, where T is a triangular matrix [23].

Adequate convergence can be achieved with bound radial basis functions of the form of exponential functions multiplied by powers of r. The resulting bound-bound matrix elements are evaluated by well-known formulas.

5 Applications

The matrix variational method has been used for calculations of electron scattering by H, Li, Na, K, He, C, N, and O atoms. In each case excellent agreement has been obtained with available experimental data and with the best results of other methods.

Calculations of inelastic e^--H scattering have been carried out primarily by Callaway and collaborators [5,24,25,26]. The ns, np degeneracy in hydrogen produces an effective static dipole potential, for inelastic scattering, that varies asymptotically

as r^{-2}. This modifies the asymptotic phase, $-\ell_p \pi/2$ in Eq. (4), so that spherical Bessel functions are no longer adequate as continuum basis functions. Seiler et al. [24,27] corrected this deficiency by including energy-dependent basis orbitals asymptotically of the form of oscillatory functions divided by powers of r.

Calculations for alkali metal target atoms [28] showed that spherical Bessel functions could be used effectively even for atoms with very strong polarization potentials.

Calculations of e^--He scattering have been carried out in three energy ranges: elastic scattering, the n=2 excitation region, and the n=3 excitation region. In the elastic scattering region, the ℓ=0 and ℓ=1 phase shifts have been determined experimentally from differential cross section measurements [29]. Figure 1 [30] shows a comparison between these experimental data, with error bars as shown, and matrix variational Bethe-Goldstone calculations (full curves) [31]. R-matrix results, which omitted the polarization potential, are shown as broken curves [32].

Calculations in the n=2 excitation region [33,34] show detailed resonance and threshold structures that are in quantitative agreement with recent experimental data [35,36].

In the n=3 region, very complex structure appears in recent experimental data, the first in which energy resolution has been reduced to 15 meV [37]. This structure is reproduced in detail by the theoretical calculations [38]. The computed total metastable production cross section ($^2S, ^2P^o$, and ^2D scattering states only) is shown in Figure 2.

Similar calculations have been carried out for target atoms C, N, and O, important in astrophysics and atmospheric physics. Very little experimental data is available for comparison, but good agreement is found between matrix variational calculations and recent calculations by the R-matrix method [6,39,40], which included pseudostates representing the full ground state electric dipole polarizability.

An important purpose of the quantitative theory is the calculation of data that cannot be obtained directly by experiment. An example is shown in Figure 3, which indicates the $^3P_2$-$^3P_1$ fine structure level collision strength for e^--O scattering, deduced from matrix variational calculations (BG) [41,42]. The comparison with full jj-coupling close-coupling results (THD) [43] is excellent. These results have been used [44] to recompute the thermal rate constant for electron cooling in the earth's ionosphere. The new cooling rate is significantly smaller than that formerly used in upper atmosphere models.

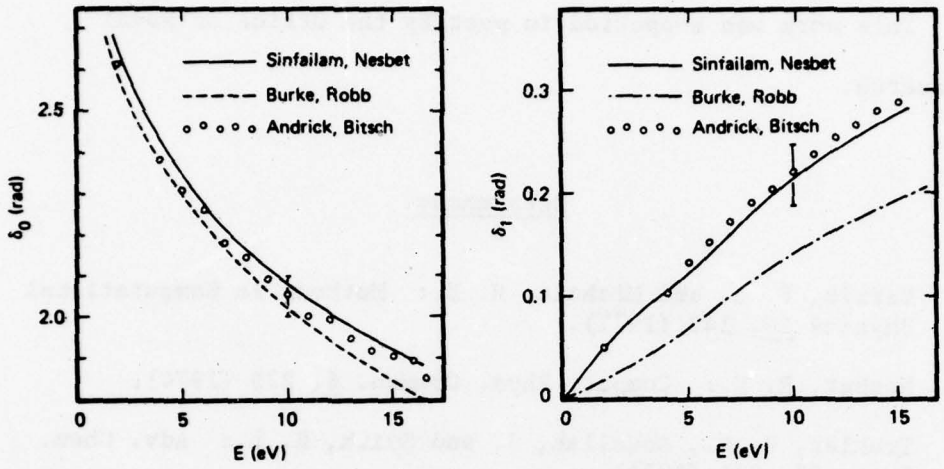

Figure 1. e-He. Comparison of elastic s- and p- wave phase shifts.

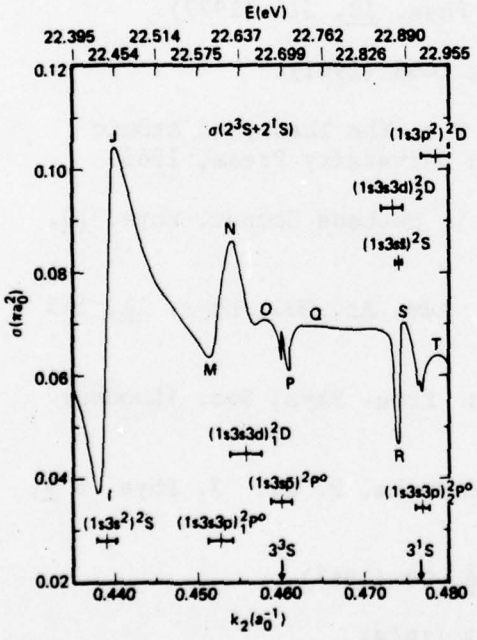

Figure 2. e-He. Computed 2^3S+2^1S excitation cross section.

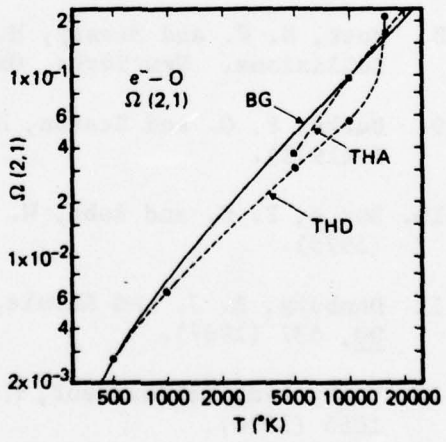

Figure 3. e-O. $^3P_2$-$^3P_1$ collision strength.

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R-MATRIX METHODS

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The procedures used in the application of R-matrix theory to atomic and molecular collision processes are presented. The computationally advantageous features of these methods are highlighted, and some applications to electron scattering and photoionization are briefly discussed.

1 Introduction

R-matrix methods have gained popularity in application to atomic physics problems only during the past decade, although they have played a prominent role in the theoretical treatment of nuclear reactions since the 1930's. Perhaps it was the fact that nuclear applications of R-matrix theory were often semi-empirical in nature that delayed their due consideration by ab initio atomic and molecular theorists. The current importance of R-matrix methods in atomic physics was highlighted during a symposium at the last ICPEAC meeting. The five invited papers [5] on the topic contain the latest and most complete review of the subject.

The central feature of R-matrix theory is illustrated in Fig. 1 by the division of the configuration space of the colliding particles into two physically distinct regions.

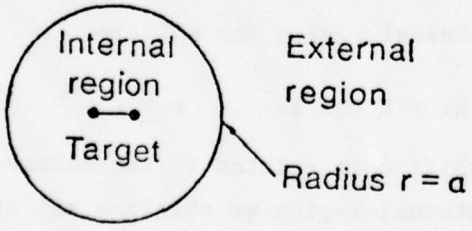

Fig. 1. Separation of configuration space.

The inner region contains the particles when they are close to the collision center. In this way the most mathematically complex part of the interaction is isolated to a finite region of configuration space, and the collision wave function therein can be expressed in terms of a discrete, complete set of basis functions. In the outer infinite region the collision wave function has its asymptotic form and can be obtained directly from the asymptotic Schroedinger equation. To obtain the scattering matrix these wave functions are linked on the boundary surface, through a quantity called the R-matrix.

In the following sections we will set up the various mathematical treatments that have been proposed within this overall concept and compare their mathematical and computational facets.

2 Formulation for Potential Scattering

Many of the mathematical features of R-matrix theory can be illustrated by consideration of a single-channel potential scattering problem. For s-wave scattering by a short-range central potential V(r) the Schroedinger Equation is

$$\left(\frac{d^2}{dr^2} + V(r) + k^2\right) F(k^2,r) = 0 \qquad (2.1)$$

Let us assume that it is an excellent numerical approximation to put V(r) = 0 for values of r greater than some radius a. The spherical surface r = a defines the R-matrix boundary. Clearly in the external region the solution is

$$F(k^2,r) = \sin kr + K \cos kr \qquad r \geq a \qquad (2.2)$$

where the phase shift δ is related to the unknown K-matrix by $K = \tan \delta$. In the internal region we obtain a set of functions $u_\lambda(r)$ as solutions of

$$\left(\frac{d^2}{dr^2} + V(r) + k_\lambda^2\right)u_\lambda(r) = 0 \tag{2.3}$$

satisfying the R-matrix boundary conditions

$$u_\lambda(0) = 0$$

$$\frac{a}{u_\lambda(a)} \cdot \left.\frac{du_\lambda}{dr}\right|_{r=a} = b \text{ (an arbitrary constant)} \tag{2.4}$$

Equations (2.3) and (2.4) satisfy Sturm-Louisville conditions, and thus the functions $u_\lambda(r)$ constitute a complete discrete set in the region $0 \leq r \leq a$. We may therefore expand the solution of Eq. (2.1) as:

$$F(k^2,r) = \sum_{\lambda=1}^{\infty} A_\lambda(k^2)u_\lambda(r) \qquad 0 \leq r \leq a \tag{2.5}$$

To obtain the coefficients $A_\lambda(k^2)$ we consider Eqs. (2.1) and (2.3), multiply them by u_λ and F, respectively, and integrate their difference to obtain

$$\int_0^a \left(u_\lambda \frac{d^2F}{dr^2} - F \frac{du^2_\lambda}{dr^2}\right) dr = (k_\lambda^2 - k^2)\int_0^a u_\lambda F \, dr \tag{2.6}$$

The left hand side of this equation can be evaluated by Green's Theorem to give:

$$\left.\left(u_\lambda(r) \frac{dF(k^2,r)}{dr} - F(k^2,r) \frac{du_\lambda}{dr}\right)\right|_{r=a} = (k_\lambda^2 - k^2)\int_0^a u_\lambda F \, dr \tag{2.7}$$

From this equation one finds immediately that should we replace F and k^2 by $u_{\lambda'}$ and $k^2_{\lambda'}$, where $\lambda \neq \lambda'$, then the l.h.s. is zero due

to Eq. (2.4) and thus the set of functions u_λ are mutually orthogonal, and can be normalized to satisfy

$$\int_0^a u_\lambda(r)\, u_{\lambda'}(r)\, dr = \delta_{\lambda\lambda'} \tag{2.8}$$

Returning to Eq. (2.7) we have that

$$A_\lambda(k^2) = \int_0^a u_\lambda\, F\, dr = \frac{1}{a} \cdot \frac{u_\lambda(a)}{k_\lambda^2 - k^2} \left[a \frac{dF}{dr} - bF \right]_{r=a} \tag{2.9}$$

If we now define the R-matrix by

$$R(k^2) = \frac{1}{a} \sum_{\lambda=1}^{\infty} \frac{[u_\lambda(a)]^2}{k_\lambda^2 - k^2} \tag{2.10}$$

then according to Eqs. (2.5) and (2.9)

$$R(k^2) = F(k^2,a) \cdot \left(a \frac{dF(k^2,r)}{dr} - bF(k^2,r) \right)_{r=a}^{-1} \tag{2.11}$$

Equations (2.10) and (2.11) give us two independent expressions for the R-matrix. Equation (2.10) says that it can be expressed in terms of quantities determined solely from properties of the basis set in the internal region. Further it says that the interaction in this region can be described solely in terms of eigenenergies and surface amplitudes, without requiring explicit knowledge of the wave function, and that the energy of interaction can be factored out in a simple and explicit way. Equation (2.11) gives us another expression for the R-matrix in terms of the exact solution on the boundary. We can therefore use (2.10) to obtain a value for R on the l.h.s. of (2.11) and then use Eq. (2.2) to obtain

$$K = \tan \delta = \frac{-\sin ka + R(ka \cos ka - b \sin ka)}{\cos ka + R(ka \sin ka + b \cos ka)} \tag{2.12}$$

which can be rewritten as

$$\tan(\delta + ka) = \frac{kaR}{1 + Rb} \tag{2.13}$$

Thus once we have R, the K matrix, phase shift and related cross section can be easily determined.

Pictorially we see that in the R-matrix treatment we have replaced the continuum spectrum of the whole of configuration space, Fig. 2a, by the discrete spectrum, Fig. 2b, in the internal region.

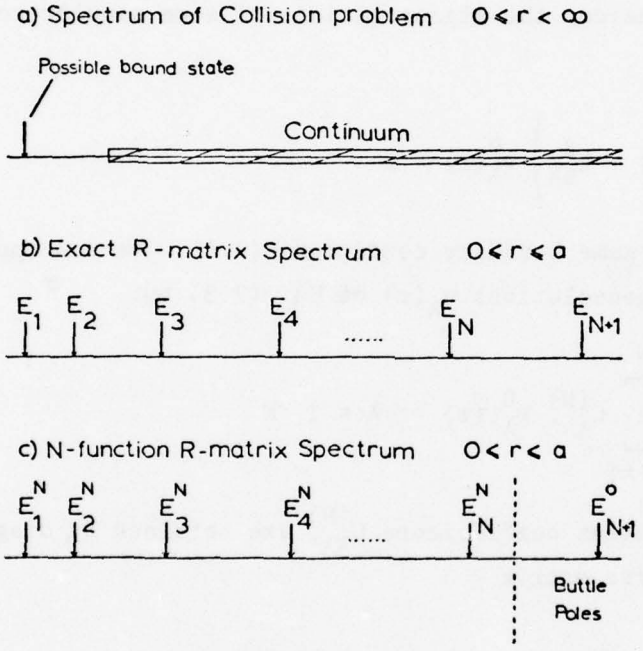

Fig. 2. R-matrix energy spectra.

3 Computation of the R-matrix

The main problem now is how to compute the R-matrix given by Eq. (2.10). Clearly we cannot deal with an infinite, albeit discrete, set of functions, and so as in most other atomic and molecular computations we have to obtain a finite representation of that set. In addition, it is not usually possible to solve the original Schroedinger equation exactly and so we must use

basis sets which satisfy some lower order, but physicaly significant, equation. The discussion in this section relates to these two problems and provides us an introduction to the practicalities of solving the multichannel problem.

Two approaches have been adopted, the first has obvious appeal to numerical integrators of coupled equations, while the second is a more natural approach for analytic basis set manipulators.

3a Expansion in an Orthogonal R-matrix Basis

Let us consider the eigensolutions of some simpler zero-order equation:

$$\left(\frac{d^2}{dr^2} + V_0(r) + k_{0\lambda}^2\right) V_\lambda^0(r) = 0 \tag{3.1}$$

subject to the same boundary conditions (2.4). We now approximate *the first N eigensolutions* $u_\lambda(r)$ *of Eq.* (2.3) by:

$$u_\lambda^{(N)}(r) = \sum_{\lambda'=1}^{N} C_{\lambda\lambda'}^{(N)} V_{\lambda'}^0(r) \qquad \lambda = 1, N \tag{3.2}$$

where the expansion coefficients $C_{\lambda\lambda'}^{(N)}$ are obtained by diagonalizing the symmetric matrix

$$H_{\lambda\lambda'}^{(N)} = -\int_0^a V_\lambda^0 \left(\frac{d^2}{dr^2} + V(r)\right) V_{\lambda'}^0 \, dr \qquad \lambda, \lambda' = 1, N \tag{3.3}$$

In matrix notation we can write

$$\underset{\sim}{C}^{(N)^T} \underset{\sim}{H}^{(N)} \underset{\sim}{C}^{(N)} = \underset{\sim}{k}^{(N)^2} \tag{3.4}$$

where $\underset{\sim}{k}^{(N)^2}$ is diagonal.

We now proceed by augmenting the N functions $u_\lambda^{(N)}(r)$ with the zero-order functions $V_\lambda^0(r)(\lambda = N + 1, \infty)$. For convenience we denote this whole set by $u_\lambda^{(N)}(r)$ and expand for the exact solution as:

$$F^{(N)}(k^2,r) = \sum_{\lambda=1}^{\infty} a_\lambda^{(N)}(k\ )\ u_\lambda^{(N)}(r) \tag{3.5}$$

The analysis proceeds as for Eqs. (2.6) through (2.11) where now we assume that the operator $\frac{d^2}{dr^2} + V(r)$ is diagonal in our basis $u_\lambda^{(N)}(r)$. This assumption introduces some error which however becomes small as N becomes large provided V_0 is chosen appropriately.

In practice the contribution from the R-matrix poles $\lambda = N + 1, \infty$ is added in by the procedure due to Buttle [6]. Since the zero-order Eq. (3.1) can be solved exactly at the energy k^2, with solution V^0, we can write the exact expression for the R-matrix from Eq. (2.11) as

$$R^0 = \left[\frac{a}{V^0(a)} \left.\frac{dV^0}{dr}\right|_{r\,=\,a} - b\right]^{-1} \tag{3.6}$$

and the contribution from the poles $\lambda = N + 1, \infty$ is

$$R_C^{0(N)} = R^0 - \frac{1}{a}\sum_{\lambda=1}^{N} \frac{V_\lambda^{0^2}(a)}{k_{0\lambda}^2 - k^2} \tag{3.7}$$

This gives the total R-matrix within the representation of states $u_\lambda^{(N)}(r)$ as:

$$R^{(N)} = \frac{1}{a}\sum_{\lambda=1}^{N} \frac{\left[u_\lambda^{(N)}(a)\right]^2}{k^{(N)^2} - k^2} + R_C^{0(N)} \tag{3.8}$$

The effect of this finite set diagonalization is shown in Fig. 2c. The Hylleraas-Undheim Theorem tells us that the pole positions in Figs. 2b and 2c must satisfy

$$k_\lambda^{(N)^2} \geq k_\lambda^2 \tag{3.9}$$

Clearly the lowest $k_\lambda^{(N)^2}$ will converge on k_λ^2 fastest with increasing N, and so incident energies in their neighborhood will be best represented for small N values. From Eqs. (3.8) and (3.9) we see that $R \geq R^{(N)}$ and so from Eq. (2.13) the approximate phase shift δ^N approaches the exact phase shift δ from below. Such effective minimum principles in the orthogonal basis R-matrix methods are discussed in greater detail by Burke and Robb [3].

3b Expansion in an Arbitrary Basis Set

It is clear that the computation of the R-matrix in the region $0 \leq r \leq a$ as described above has many features of obtaining bound state configuration interaction wave functions. Namely, one has to compute a Hamiltonian matrix H in terms of some effectively finite range basis. When one comes to considering such a complex problem as electron-molecule scattering it would be foolish not to take advantage of the available bound state software available to evaluate Hamiltonian matrices in terms of arbitrary Slater-type-orbital (STO) of Gaussian-type-orbital (GTO) bases. We therefore consider the expansion of $F(k^2,r)$ in (1) in terms of such a basis set.

Bloch [2] has shown that the operator

$$\frac{d^2}{dr^2} + V(r) + L_b \tag{3.10}$$

where

$$L_b = \delta(r - a)\left[\frac{d}{dr} - b\right] \tag{3.11}$$

is Hermitian in the region $0 \leq r \leq a$ with respect to an arbitrary set of functions. We therefore introduce a complete set of functions u_λ satisfying

$$\left(\frac{d^2}{dr^2} + V(r) + L_b + k_\lambda^2\right) u_\lambda(r) = 0 \qquad (3.12)$$

These functions $u_\lambda(r)$ may be expanded in terms of arbitrary functions, since the Bloch operator L_b guarantees that the $u_\lambda(r)$ satisfy the boundary condition (2.4) even though the expansion functions do not. We may then proceed as in the previous section to evaluate the R-matrix and phase shift.

In contrast to the method described in ¶3a the present approach may not require the inclusion of a contribution from distant levels to obtain reasonable convergence. The arbitrary basis can be chosen essentially to cover the whole interior configuration space and so the idea of "nearby" or "distant" levels is essentially lost.

4 Multichannel Electron-Atom and Electron Molecule Scattering Considerations

4a The Methods

The most important and most difficult effects to be allowed for in the interaction of an electron with an N-electron atom are electron-electron exchange and correlation. For the total (N + 1) electrons these occurs within the effective radius a of the charge distribution of the N-electrons. Outside this radius the scattered electron experiences only Coulomb and/or multipole moment and centrifugal terms in the interaction. Since these are reasonably weak and well behaved, solutions for $r \geq a$ can easily be obtained at most incident electron energies.

In the internal region, from what has been said above, we ideally should use bound-state configuration interaction type wave functions to deal with electron-electron exchange and correlation. Generalizing our earlier discussion of potential scattering we define a basis set of functions within each πLS of the (N + 1) electron system as

$$\Psi_k = A \sum_{i\lambda} a_{i\lambda k} \Phi_i V_\lambda^0(r) + \sum_j b_{jk} \chi_j \qquad (4.1)$$

where the Φ_i are functions representing the real- or pseudo-target states of interest coupled with functions representing the spin and angular motion of the scattered electron. The target states themselves may be represented by C.I. functions constructed from a bound orbital basis. The V_λ^0 are solutions of Eq. (3.1) with some appropriate zero-order potential, usually the static potential of the target ground state. They represent the radial motion of the scattered electron for $0 \leq r \leq a$, and are generated to be orthogonal to the bound orbitals of the same orbital angular momentum. A is the antisymmetrization operator which properly antisymmertrizes the (N + 1)-electron orbitals. The functions χ_j are (N + 1)-electron functions constructed from the bound orbital basis alone. They are included to complete the function space omitted by orbital orthogonality in the first term of Eq. (4.1), and to allow for further electron-electron correlation.

Since the basis orbitals satisfy the boundary conditions (2.4) they form a complete discrete set of functions, along with the bound orbitals, for each channel angular momentum ℓ. The functions Ψ_k are therefore a complete set of (N + 1)-electron functions and we may expand the wave function at any energy E as

$$\Psi_E = \sum_k A_{Ek} \Psi_k \qquad (4.2)$$

We obtain the A_{Ek} by substituting Ψ_E into the Schroedinger equation

$$(H^{N+1} - E)\,\Psi_E = 0 \tag{4.3}$$

and writing a Greens equation similar to Eq. (2.6). Use of the boundary condition (2.4) and the fact that all relevant integrals reduce to those in the r_{N+1}th coordinate (since this is the only coordinate with finite surface terms) yields the multichannel forms of Eqs. (2.10) and (2.11) i.e.,

$$R_{ij}(E) = \frac{1}{2a} \sum_k \frac{W_{ik}(a)\, W_{jk}(a)}{E_k - E} \tag{4.4}$$

and

$$F_{ij}(E,a) = \sum_n R_{in}(E) \left(a \frac{dF_{nj}(E,r)}{dr} - b_n F_{nj}(E,r) \right)_{r=a} \tag{4.5}$$

where

$$W_{ik}(a) = \sum_\lambda a_{i\lambda k}\, V_\lambda^0(a) \tag{4.6}$$

The main problem remaining is the calculation of the Ψ_k and E_k. These quantities allow us to define the R-matrix by Eq. (4.4) and from Eq. (4.5) we obtain the multichannel K-matrix given by the wave function in the external region. Methods for determining this wave function have been adequately discussed [17] and programmed [18] by Norcross.

Two approaches have principally been used in atomic physics to obtain Ψ_k and E_k. In the first, adopted by Burke et al. [3] the Hamiltonian is divided into two parts

$$H^{N+1} = H_0 + H_{int} \tag{4.7}$$

where H_0 defines a zero-order potential problem in each channel, as per equation (2.1), which can be used to determine the orbitals $V_j^0(r)$. The coefficients $a_{i\lambda k}$ and b_{jk}, and eigenvalues E_k are determined by diagonalizing the Hamiltonian matrix:

$$(\Psi_k|H^{N+1}|\Psi_{k'}) = E_k\ \delta_{kk'} \tag{4.8}$$

Important advantages of this method are (a) that a single matrix diagonalization determines the R-matrix at all energies E, and (b) that it contains a soluble zero-order Hamiltonian which can be used to obtain a Buttle correction (see ¶3a) to the diagonal R-matrix elements.

The second approach, which has been applied to electron-molecule scattering by Schneider [23] and Burke et al. [4], uses analytic continuum basis orbitals together with a multichannel Bloch operator:

$$L_b = \frac{1}{2}\sum_i |\Phi_i > \delta(r - a)\left(\frac{d}{dr} - \frac{b_i}{a}\right)<\Phi_i| \tag{4.9}$$

which is added to the total Hamiltonian for the system, to provide a Hermitian operator. Schneider and coworkers use a GTO basis in prolate spheroidal coordinates whereas Burke and coworkers use an STO basis on the nucleii and the center of mass of the target. The main advantage of these approaches is that analytic integrals can be performed rapidly, however, it is not clear as yet that in problems which involve several electronic states and/or significant electronic interchannel coupling, that such arbitrarily chosen bases will have satisfactory convergence and linear-independence properties.

Two other methods have been applied to limited cases in atomic physics. Fano and Lee [11] and Lee [14] have used an

eigenchannel approach to study the $e^- + Ar^+$ interaction in the photonionization of Ar. This method essentially adjusts the boundary conditions (2.4) in each channel so that an eigenvalue E_k falls at the energy E of interest. Shimamura [24] has indicated how this approach might be extended to problems with long-range potentials. Oberoi and Nesbet [19] have used another approach which essentially rewrites the equation for the A_{Ek} as a set of linear equations at each energy E. Since the solution of a set of linear equations is much more rapid than the diagonalization of a matrix of equivalent dimension, this method may be much more rapid if only a few energies are required.

Further ideas for improving on weaknesses in the above methods have been discussed in the literature. Shimamura [5] has shown how to obtain a continuous wave function at the R-matrix boundary from quantities currently evaluated in the theory, and Zvijac et al [26] have shown how to variationally correct the lower eigenvalues E_k of Eq. (4.8) for the effect of the high lying Buttle poles neglected in the finite matrix diagonalization.

4b Computational Aspects of the Methods

The major computational task in R-matrix methods is the calculation and diagonalization of a Hamiltonian matrix. This is equivalent to the problem of configuration interaction for bound states, and so the same well-tried analytic and numerical procedures and computer codes [11, 21] can be used. The methods are also remarkably free of numerical errors which can occur in direct numerical integration of the close-coupling equations, since they deal with integrals of basis functions which can be evaluated with high precision. Further we may easily add spin-orbit terms and other relativistic terms to the Hamiltonian since only a few additional integrals need be calculated.

Some comments about the practical aspects of using the orthogonal and arbitrary basis set methods are required. The

arbitrary basis method does not build any of the physics of the problem into the basis a priori. Rather it relies on using the simultaneous diagonalization and application of the Bloch operator to obtain accurate R-matrix eigensolutions, which may not however be sequential.

In contrast the orthogonal basis method builds essential physics into the potential V_o and adds on eigensolutions sequentially. The methods therefore are analogous in character to the Multi-Configurational Hartree-Fock and Superposition of Configuration methods of bound state calculations, and it is to be expected that the arbitrary basis set should provide better lower eigensolutions than the equivalent sized orthogonal basis set. However there is danger of redundancy, linear dependence and omission of significant parts of function space in the arbitrary basis method which is not present in the orthogonal basis method.

5 Results From R-matrix Calculations

R-matrix methods have been used in atomic physics to calculate electron scattering cross-sections, dipole polarizalorities, photoionization cross sections, Van der Waals coefficients, free-free bremsstrahlung and optical harmonic coefficients. A review of this work has been given by Robb [5]. To facilitate quantitative illustration of some of the computational points discussed in the previous sections, we will restrict ourselves to these examples.

5a Elastic Scattering of Electron by Atomic Helium

Absolute values of elastic scattering phase shifts for atomic helium are required to serve as a measurement standard for future experiments. Berrington, et al. [1] have recently performed an R-matrix calculation for electron-helium scattering in which they claim maximum errors of 1½% in the s-wave phase shift,

6% in the p-wave phase shift, much less than 1% in higher partial wave phase shifts, and 3% in the total and momentum transfer cross-sections at energies from 0-16 eV. To obtain these results

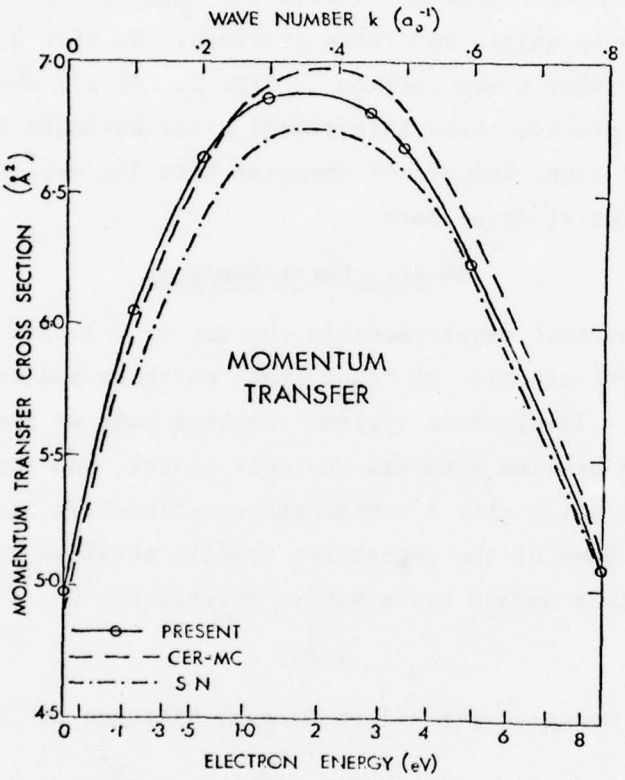

Fig. 3. Momentum transfer cross-sections for electron-helium scattering. The present results are those of Berrington et al. [1], the CER-MC curves are experimental values of Milloy and Crompton [15] and the SN curves are calculations of Sinfailam and Nesbet [25] using less accurate target wave functions.

they used a ground state wave function which gave 98% of the ground state correlation energy, together with 2 ^{1}P and 3 ^{1}D pseudostates which gave the exact ground state dipole and quadrupole polarizabilities. In addition they added 104 and 196 of the three electron χ_j functions of Eq. (4.1) in the ^{2}S and ^{2}P° symmetries, respectively, to allow as completely as possible for higher

channel couplings. Further, they adjusted the logarithmic derivative b_i in each channel to give most rapid convergence of the R-matrix basis set. Using the minimum principle discussed above and fitting of the phase shifts to effective range formulae, they are able to make estimates of both the magnitude and sign of the error in phase shifts and cross sections. We show a plot of the momentum tranfer cross section in Fig. 3. At all the energies where they provide their theoretical error estimate they obtain the correct sign, and at all energies they lie well within the ±2% experimental error bars.

5b Attachment Energies

An important development in the use of R-matrix theory has been the determination of bound state energies and wave functions for the (N + 1)-electron system. In this case we run the code as a collision problem with all channels closed, and look for the eigenvalues which give a continuous wave function at the R-matrix boundary. Some of the impressive results obtained by LeDourneuf [12] with this method are given in Table I for C^-, N^-, and O^-.

TABLE I

Attachment Energies (in eV) of Cargon, Nitrogen and Oxygen Atoms

	C^-		N^-	O^-
	$^4S^o$	$^2D^o$	$^3P^e$	$^2P^o$
Experiment	1.262	.035	-.050±.050?	1.462
R-matrix	1.228	.001	0.004	1.412
H.F	.550		-2.150	-0.542
B.G.	1.211	-.275	-0.582	0.963
S.O.C.	1.11		-0.52	1.13

This table clearly shows the limitations of the standard structure methods, such as Hartree-Fock (H.F.) [8], Bethe-Goldstone (B.G.) [16] and Superposition of Configurations (S.O.C.) For

example, the most extensive S.O.C. calculations of Sasaki and Yoshimine [22], which includes as many as 2649 configurations for O^-, has an error of 0.33 eV for O^- and nearly 0.5 eV for N^-. The R-matrix method, which is basically a collisional approach, concentrates directly on the energy difference between the target ground state and negative ion ground state, and in all cases is in reasonable agreement wth experiment.

5c Photoionization of Atomic Aluminum

An important consequence of the last section is that for photoionization one can evaluate both the bound and continuum wave functions within the electron-plus-residual-ion framework, with the same basis functions, and thus treat both on the same footing (i.e., with the same correlation effects in both). In this way we can obtain accurate ionization threshold energies, and thus resonance positions, and can include the amount of correlation required to obtain good agreement between the length and velocity forms of the cross section. A particularly sensitive case is the open-shell atom Aluminum. For this case there is considerable configuration interaction in both the N- and (N + 1)-electron systems. In Fig. 4, we show the length photoionization spectrum from the R-matrix calculation of Le Dourneuf, et al. [13] compared with the experimental spectrum of Esteva, et al. [9]. The absolute magnitudes of the cross sections, not compared here, lie within a few percent of one another. It should be noted that the R-matrix calculation accurately represents the $^2D^e$ autoionization spectrum which is strongly perturbed by correlation χ_j functions such as $1s^2\ 2s^2\ 2p^6\ 3s\ 3p^2\ ^2D^e$.

7 Concluding Remarks

We can definitely say that R-matrix methods are an established useful tool for solving atomic scattering problems. However, these methods are still far from their final development. All of the above discussion has involved the solution of

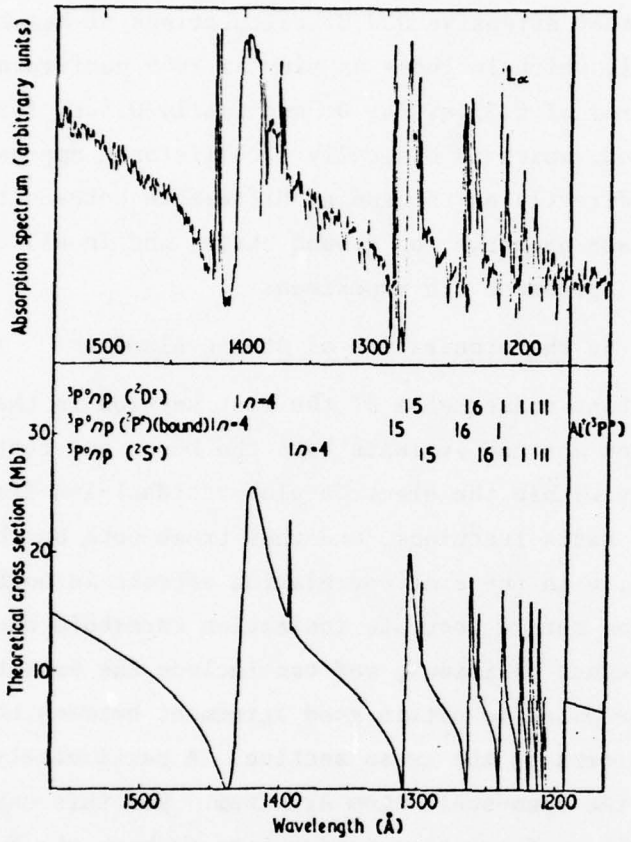

Fig. 4. Comparison of the length photoionization cross-section of LeDourneuf et al. [13] with the experimental results of Esteva et al. [9]. The energy scale has been adjusted so that the theoretical and experimental $Al^+(^3P^o)$ thresholds coincide.

coupled-channel problems in terms of uncoupled-channel bases. Many coupled-channel zero-order problems are extremely tractable to solution, e.g., the no-exchange close-coupling equations, and could possibly provide much more rapidly convergent bases than those tried so far.

There is also the problem of two low energy electrons in the continuum. An R-matrix calculation should be particularly appropriate for this problem since the two electrons correlate with

the other electrons only when they are within the residual ion charge cloud, and outside of this region a correlated asymptotic form of their wave function has been discussed by Peterkop [20]. This subject has been discussed further by Fano and Inokuti [10].

Acknowledgements

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ASYMPTOTIC COMPLETENESS FOR QUANTUM SCATTERING

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We give a new proof of asymptotic completeness for potential scattering and for two-cluster rearrangement collisions. The allowed interactions include short range- and Coulomb- forces.

The dynamics are given by a Hamiltonian $H=H_o + V + v$ with $H_o = -\frac{1}{2}\Delta$. The short range potential V may be singular and velocity-dependent, it obeys

$$\|V\psi\| \leq a\|H_o\psi\| + b\|\psi\| \quad \forall\ \psi\in\mathcal{D}(H_o), a<1;$$

$$\|V(H_o+1)^{-1} F(|\vec{x}|\geq R)\| =: h(R)\in L^1([0,\infty),dR);$$

where F(.) projects onto states localized in the indicated region; e.g. a $|\vec{x}|^{-1-\varepsilon}$ decay of V is allowed. $v(\vec{x}) = e(1+|\vec{x}|^2)^{-\frac{1}{2}}$ describes the long range part of the Coulomb interaction $(e/|\vec{x}|-v(\vec{x}))$ is of type V).

The (modified) free time evolution[1] is

$$U_o(t) = \exp - i(H_o t + \int_o^t dt' v(\vec{p}t'))$$

which coincides with $\exp -iH_o t$ if $v=0$, i.e. Coulomb forces are absent. The (modified)wave operators are then

$$\Omega_{\pm} = \text{s-lim}_{t\to\pm\infty} \exp(iHt)U_o(t)$$

(see [5] for notation and details.)

For potential scattering - or equivalently two-particle scattering - we show asymptotic completeness in its strong form: all states orthogonal to the bound states ($H_{pp}^{\perp}$) lie in the range of both (modified) wave operators $\Omega_{\pm}$, i.e. they evolve asymptotically free in the future and past. The absence of a singular continuous spectrum in the Hamiltonian is an immediate corollary.

The method of proof consists in following with mathematical rigour the intuitive reasoning of a physicist [2,3]: A state which stays always within a finite distance from the center of the potential is a bound state (lies in H_{pp}). A state with

continuous energy distribution instead will be arbitrarily far away from the potential for suitably chosen very late and early times. From then on classical physics prevails: we decompose the state into its incoming and outgoing components by simultaneously restricting the momenta and the position (the latter only approximately to comply with the uncertainty principle): the part of $\Phi_{out}(\Phi_{in})$ localized around $\vec{a}$ does not contain any momenta with directions around $-\vec{a}$ $(\vec{a})$. A classical free particle with this phase space distribution moves in the future (past) along trajectories far away from the center of the potential, the distance increases asymptotically linear in time (if one avoids very small momenta by a density argument). The same is true in good approximation for a quantum particle moving under the free or modified free evolution $U_o(t)$. Thus the phase space decomposition of the far out localized states allows to estimate the space-time-behavior in the future (past).

Along these trajectories a particle should not feel the short range potential, indeed $(\Omega_- - 1)$ which measures the amount of interaction in the future is small on Φ_{out} (similarly $(\Omega_+ - 1)\Phi_{in} \approx 0$).

If Coulomb forces are present one more step is necessary. The modified free evolution $U_o(t)$ is a good approximation of $\exp(-iHt)$ only if $\vec{x} \approx \vec{p}t$. To control this one has to wait a second time while the state evolves under an intermediate position- and momentum-dependent potential $v(\vec{a} + \vec{p}t)$ which approximates the action of $v(x)$ on the component of the state localized around $\vec{a}$. Some time $\vec{p}t$ will dominate over all $\vec{a}$ that occur, from then on $(\Omega_- - 1)\Phi_{out}$ is small $((\Omega_+ - 1)\Phi_{in} \approx 0)$. Clearly Φ_{out} lies in the range of the outgoing wave operator Ω_- and Φ_{in} in Ran Ω_+. A little extra argument shows that Φ_{in} vanishes in the far future and Φ_{out} in the far past, this completes the proof of

THEOREM 1. The wave operators $\Omega_\pm$ are complete.

In N-body scattering one often finds an energy interval (Σ_2, Σ_3) where breakup into two clusters is possible, but three

independent subsystems cannot be formed (e.g. low energy e^--He^+-scattering). Without significant changes our method allows to treat the scattering of two bounded subsystems like that of two particles, even if both of them are charged.

Let α denote the channel, i.e. it specifies the breakup into two clusters and the particular bound state of each subsystem. With V_{ij} and ν as before the Hamiltonian is

$$H = H_o + \sum_{i<j}(V_{ij}(\vec{x}_i-\vec{x}_j) + e_i e_j \nu(\vec{x}_i-\vec{x}_j)).$$

H_α omits in H all potentials connecting the two subsystems, $\vec{p}_\alpha$ is the relative momentum of the centers of mass of the subsystems, and g_α is the product of the total charges of the two clusters. The (modified) free channel evolution is

$$U_\alpha(t) = \exp -i(H_\alpha t + g_\alpha \int_o^t dt' \, \nu(\vec{p}_\alpha t')).$$

Let Π_α denote the projection onto those states which are composed of the corresponding bound states of the subsystems. We have [4]

THEOREM 2: $\Omega_{\alpha\mp} = \lim_{t\to\pm\infty} \exp(iHt)U_\alpha(t)\Pi_\alpha$ exist and are complete below the three - cluster - threshold, i.e. the range of $\oplus_\alpha \Omega_{\alpha\mp}$ contains all states with continuous energy distribution below Σ_3.

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ANALYTIC MULTICHANNEL PROJECTIONS

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If the interaction in a multiparticle system depends analytically on complex particle coordinates $xe^{-i\phi}$, the usual Hamiltonian $H(0)$ can be continued to yield Hamiltonians $H(\phi)$ with $\phi \neq 0$. The continuous spectrum of $H(\phi)$ consists of a set of half-lines starting at the thresholds λ_a of the scattering channels a and making angles 2ϕ with the positive real axis [2,3]. Associated with each channel is an idempotent operator $P_a(\phi)$ projecting onto an invariant subspace of $H(\phi)$ [1,4].

For smooth interactions in the Schmidt class, the operator

$$U_a(t,\phi) = P_a(\phi) \exp \{i[H(\phi) - \lambda_a]te^{-2i\phi}\} \tag{1}$$

is bounded uniformly in t. There exist wave operators $W_a(\pm\infty,\phi)$. The projection $P_a(\phi)$ can be written as

$$P_a(\phi) = W_a(\infty,\phi)W_a^*(\infty,-\phi) = W_a(-\infty,\phi)W_a^*(-\infty,-\phi) \ . \tag{2}$$

The operators $P_a(\phi)$ and $W_a(\pm\infty,\phi)$ transform analytic functions of $xe^{-i\phi}$ into analytic functions.

In Eqs. (1) and (2), it is assumed that $\phi > 0$. To discuss the limit of ϕ tending to 0, it is convenient to begin with the lowest threshold. Let this be λ_1. If t tends to $-\infty$, the operator

$$\sum_a P_a(\phi) \exp \{i[H(\phi) - \lambda_1]te^{-2i\phi}\} \tag{3}$$

tends to $U_1(t,\phi)$ plus a sum of exponentially decreasing terms. It is due to this that the operator $W_1(-\infty,\phi)$ has a limit $W_1(-\infty,+0)$. This is the wave operator $\Omega_1(-\infty)$ of physics. Similarly, $W_1(\infty,-\phi)$ tends to $\Omega_1(\infty)$, but the reasoning does not apply to

$W_1(\infty,\phi)$ and $W_1(-\infty,-\phi)$.

Owing to Eq. (2),

$$\begin{aligned} &\text{Range } P_1(\phi) = \text{Range } W_1(-\infty,\phi) , \\ &\text{Null space } P_1(\phi) = \text{Null space } W_1^*(\infty,-\phi) . \end{aligned} \tag{4}$$

Since $P_1(\phi)$ is a projection, it follows that

$$\text{Null space } W_1^*(\infty,-\phi)W_1(-\infty,\phi) = \emptyset . \tag{5}$$

Since $P_1^*(\phi)$ is also a projection,

$$\text{Null space } W_1^*(-\infty,\phi)W_1(\infty,-\phi) = \emptyset . \tag{6}$$

The analyticity properties of the operators W now imply that

$$\text{Null space } \Omega_1^*(\infty)\Omega_1(-\infty) = \text{Null space } \Omega_1^*(-\infty)\Omega_1(\infty) = \emptyset . \tag{7}$$

The result (7) is necessary and sufficient in order that there exists a projection with the same range as $\Omega_1(-\infty)$ and the same null space as $\Omega_1^*(\infty)$. This projection is the limit of $P_1(\phi)$ as ϕ tends to 0 through positive values. Specifically,

$$P_1(+0) = \Omega_1(-\infty)[\Omega_1^*(\infty)\Omega_1(-\infty)]^{-1}\Omega_1^*(\infty) . \tag{8}$$

The operator $P_1(-\phi)$ equals $P_1^*(\phi)$ and tends to the operator $P_1^*(+0)$, which may also be denoted by $P_1(-0)$.

Now let there be N channels, the thresholds satisfying $\lambda_1 < \lambda_2 < \cdots < \lambda_N$. Write

$$Q_b(\phi) = I - \sum_{a<b} P_a(\phi) . \tag{9}$$

It can be shown by induction that

$$\lim_{\phi \to +0} W_b(-\infty, \phi) = Q_b(+0)\Omega_b(-\infty) , \tag{10}$$

and similarly for the limit of $W_b(\infty,-\phi)$. Also,

$$\lim_{\phi \to +0} P_b(\phi) = Q_b(+0)\Omega_b(-\infty)[\Omega_b^*(\infty)Q_b(+0)\Omega_b(-\infty)]^{-1}\Omega_b^*(\infty)Q_b(+0). \tag{11}$$

If a wave function is orthogonal to the ranges of the operators $\Omega_a(-\infty)$ $(a = 1,2,\ldots,N)$, it is orthogonal to the ranges of the projections $P_a(+0)$. Since the orthogonal complement of $\Sigma_{a=1}^{N} P_a(\pm 0)$ is the projection onto the space spanned by the eigenfunctions of any bound states, it follows that the system has the property of asymptotic completeness.

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ANALYTIC CONTINUATION OF ATOMIC SCATTERING AMPLITUDES

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Consider the case of non-relativistic atomic scattering from an initial channel i to a final channel f where each of the channels corresponds to two clusters, at least one of which is neutral. Let ψ^i, V^i (ψ^f, V^f) be the state and inter-cluster potential in channel i(f) respectively. Then a formal expression for the scattering amplitude $\overline{T}_{fi}(E)$ is given by $\overline{T}_{fi} = T^o_{fi}(E) + T_{fi}(E)$, where $T^o_{fi}(E) = (\psi^f | V^i \psi^i)$ is the Born term and

$$T_{fi}(E) = \lim_{\varepsilon \downarrow 0} (\psi^f | V^f (E + i\varepsilon - H)^{-1} V^i \psi^i) \qquad (1)$$

in the usual notation. We consider the question of the existence of the limit in (1) and of the on-shell analytic continuation of $T_{fi}(E)$ to the second sheet. The poles of $T_{fi}(z)$ on the second sheet are defined to be the resonance points. These are expected to be in a one to one correspondence with the complex eigenvalues of the rotated Hamiltonian.

Existence of $T_{fi}(E)$ We restrict ourselves to the case of a fixed partial wave and prove the existence of the on-shell scattering amplitude under the following additional conditions:

i) The energy E is below any three cluster threshold.

ii) For every channel corresponding to two clusters that is open in the energy range being considered, at least one cluster is neutral.

A proof of existence is provided within the framework of the analytic Fredholm theory [1]. We begin with the Weinberg-Van Winter equation for the resolvent and separate from its kernel and the inhomogeneous term the parts that are singular in the energy range being considered and thus obtain a set of coupled-channel integral

equations

$$u_n(z) = \alpha_n(z) + \sum_{m=1}^{j_o} A_{nm}(z)\, u_m(z), \quad n = 1,\ldots,j_o \qquad (2)$$

$T_{fi}(z)$ is given by $T_{fi}(z) = (v_n, u_n(z))$ where v_n, $u_n(z) \in L^2(R^3)$ for Im $z \neq 0$. Here $\alpha_n(z)$ is a well behaved family of vectors in $L^2(R^3)$ and $A_{nm}(z) = B_{nm}(z)\, \mathcal{K}_m(z)$ where $\mathcal{K}_m(z)$ is a family of compact operators involving only a two body Green's function and $B_{nm}(z)$ is a "pseudo-local effective potential" linking the channels m and n. This means, roughly, that $B_{nm}(z)$ is an integral operator with kernel $b_{nm}(z, r_n, r'_m)$ which decays exponentially for large $|r_n - r'_m|$. This property is shown to be implied by the boost analyticity of H.[2]. This reduces the problem to a coupled-channel two-body problem which can be solved by a standard procedure.

Analytic Continuation To continue the on-shell partial wave amplitudes we follow the procedure outlined in [3]. For example, assuming all bound states are S-wave, the S-wave projection of (2) becomes, in momentum space,

$$(p|u_n) = (p|\alpha_n) + \sum_{m=1}^{j_o} \int_o^\infty dq \int_o^\infty dq' (p|B_{nm}|q)(q|\mathcal{K}_m|q')(q'|u_m) \qquad (3)$$

The idea is to distort the integration contours as p_i, p_f, the initial, final momenta, become complex, in such a way that the appropriate contours always pass through p_i, p_j. The key point is to demonstrate the necessary analyticity of the kernel of (3). For $(q|\mathcal{K}_m|q')$ this is straightforward, and our attention is concentrated on $(p|B_{nm}|q)$. We write

$$(p|B_{nm}|q) = \int d\underline{r} \int d\underline{r}'\, r^{-1} \sin pr (\underline{r}|B_{nm}|\underline{r}')\, r'^{-1} \sin q\, r' \qquad (4)$$

Writing $2i \sin x = e^{ix} - e^{-ix}$ in (4) leads to four terms. Complex

scaling (with different angles of rotation) and pseudo-locality leads to the required analyticity, provided that the contours for different m lie along the same ray at infinity. This condition, together with the earlier restriction, means that in general contour distortions more complicated than rotations are required.

If, after distortion, there is a solution of the homogeneous version of (3) (usually implying a pole in the continued amplitude), further distortions may be performed without the requirement that the contours pass through p_i, and a homogeneous equation with all integrals along $p \approx te^{i\alpha}$, $0 \leq t < \infty$, obtained. In this way, a correspondence with eigenvalues of the 'rotated' Hamiltonian H_α follows.

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SOME N-BODY TRANSITION OPERATOR EQUATIONS CONTAINING CHANNEL PROJECTION OPERATORS

Colston Chandler and A.G. Gibson

Beginning with Faddeev [1], much effort has been expended in deriving equations which will reduce the N-body ($N \geq 3$) quantum scattering problem to a system of solvable (at least in principle) integral equations. An incomplete list of references is [1-7]. These equations all have some different features, but they divide into two broad classes*: (1) Those systems [1-3] which have a unique solution but, due to slow connectivity, require a large number of coupled equations, and (2) Those systems [4-7] which have a quickly connected kernel and a relatively small number of coupled equations but have spurious solutions [8,9]. A common feature of all of these equations is that the unknown quantities are operators mapping the full N-body Hilbert space $\mathcal{H}_N$ into itself. This is in spite of the well-known fact that all that is really needed are, for example, transition operators restricted to the initial and final channel subspaces $\mathcal{H}_\alpha$ and $\mathcal{H}_\beta$, respectively.

In this note we describe some transition operator equations for nonrelativistic multichannel quantum scattering which have been derived by the authors [10]. These equations have unknown operators which act only on the channel subspaces. The key to deriving our equations is to invert the operator $JJ^* \equiv \sum_\alpha P_\alpha$, and to use its inverse

$$(JJ^*)^{-1} = m_N^{-1} \sum_{n=0}^{\infty} (I_n - m_N^{-1} \sum_\alpha P_\alpha)^n \qquad (1)$$

* An exception which has been brought to our attention by Barry Simon is the equation used by Sigal in [13]. It has both a unique solution and a compact kernel.

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in the kernel of the equations. Here $P_\alpha = \hat{P}_\alpha \otimes I_\alpha^0$ denote the orthogonal projections of $\mathcal{H}_N$ onto $\mathcal{H}_\alpha$, where $\hat{P}_\alpha$ is the projection onto the internal coordinate eigenfunctions and I_α^0 is the identity operator on the external (intercluster) coordinates. I_N is the identity on $\mathcal{H}_N$, and m_N is the number of different possible clusterings for N particles. The series in Eq. (1) is a norm convergent Neumann series.

The motivation for introducing the operator $(JJ^*)^{-1}$ would be rather difficult to see if it were not for a two Hilbert space formulation of the problem [10]. In this formulation one space is $\mathcal{H}_N$ and the other "asymptotic" space is the direct sum space $\mathcal{H} \equiv \oplus_\alpha \mathcal{H}_\alpha$. The bounded injection operator $J : \mathcal{H} \to \mathcal{H}_N$ is defined by $J \oplus_\alpha \varphi_\alpha \equiv \sum_\alpha \varphi_\alpha$, and J^* is its adjoint.

For each channel α the total Hamiltonian H_N may be written as $H_N = H_\alpha + \bar{V}_\alpha$, where H_α is the channel Hamiltonian and $\bar{V}_\alpha$ is the sum of intercluster pair potentials. Let $R_N(z) \equiv (z-H_N)^{-1}$ and $R_\alpha(z) \equiv (z-H_\alpha)^{-1}$. The N-body scattering operator S and the resolvent operator $R_N(z)$ are normally not studied directly but rather via some transition or analogous operators; e.g. it suffices (cf. [10]) to know the transition operators

$$T_{\beta\alpha}(z) \equiv P_\beta\{\bar{V}_\alpha + \bar{V}_\beta R_N(z)\bar{V}_\alpha\}P_\alpha . \tag{2}$$

As a first step, we combine our two Hilbert space formulation with the Lippmann-Schwinger method to derive the system of equations [10]

$$T_{\beta\alpha} = P_\beta \bar{V}_\alpha P_\alpha + P_\beta \bar{V}_\beta (JJ^*)^{-1} \sum_\gamma R_\gamma T_{\gamma\alpha} . \tag{3}$$

Eq. (4) applies only if all potentials are of short range. However, if some repulsive Coulomb potentials are present, then a method similar to that of Alt, Sandhas, and Ziegelmann [11] may be used to "factor out" the Coulomb contributions. Let $H_\alpha^c \equiv H_\alpha + V_\alpha^c$ where V_α^c is the sum of Coulomb interactions between clusters, and let $\bar{V}_\alpha^c \equiv H_N - H_\alpha^c$. Let $H_\alpha^D(t)$ denote Dollard's distorted channel Hamiltonians [12]. Then

$$P_\alpha^\pm \equiv \underset{t\to\pm\infty}{\text{s-lim}}\, e^{iH_\alpha^c t} P_\alpha e^{-iH_\alpha^D(t)} \tag{4}$$

exist and are of the form $P_\alpha^\pm = \hat{P}_\alpha \otimes \omega_\alpha^\pm$, where $\omega_\alpha^\pm$ are the pure Coulomb wave operators for the clusters behaving as if they were point charges. We assume that $\omega_\alpha^\pm$ are known and asymptotically complete. This assumption is known to be satisfied if only two of the particles are charged. It can be proved [10] that it is sufficient to know the transition operators

$$T_{\beta\alpha}^c(z) \equiv P_\beta^{+*}[\bar{V}_\alpha^c + \bar{V}_\beta^c R_N(z)\bar{V}_\alpha^c]P_\alpha^- \tag{5}$$

and that a system of equations for $T_{\beta\alpha}^c$ is

$$T_{\beta\alpha}^c = P_\beta^{+*}\bar{V}_\alpha^c P_\alpha^- + P_\beta^{+*}\bar{V}_\beta^c(JJ^*)^{-1}\sum_\gamma R_\gamma T_{\beta\alpha}^c . \tag{6}$$

Eq. (6) reduces the Coulomb problem to a short-range problem plus the insertion of the known operators $\omega_\alpha^\pm$. We note that if the Coulomb potentials are "shut off", then Eq. (6) reduces to Eq.(3).

The systems of equations (3) and (6) have some desirable features and some undesirable features. The abstract form of these equations is the same for all N, and they reduce to the Lippmann Schwinger equation for $N = 2$. The solution of each of these equations is unique. Since the range of $T_{\gamma\alpha}$ or $T_{\gamma\alpha}^c$ is contained in $\mathcal{H}_\gamma$, the resolvent operator $R_\gamma(z)$ is of the simple form $R_\gamma(z) = (z - \lambda_\gamma - H_\gamma^0)^{-1}$, where λ_γ is the sum of the eigenvalues corresponding to the bound states of the fragments in channel γ and H_γ^0 is the free motion Laplacian operator for the external coordinates. The P_β factors in the kernel of the equations provide some additional connectivity, and, in particular, the term $P_\beta\bar{V}_\beta$ or $P_\beta^{+*}\bar{V}_\beta^c$ is connected for all two cluster channels. However, the kernel terms for the other channels are not connected or compact even after iterating the equations.

One way of obtaining a connected kernel is to use a Weinberg-van Winter-type method on the nonconnected equations in the system (3) (or (6)). By working within our two Hilbert space formulation, this can be done systematically for all N. The resulting system for $N = 3$ is [10]

$$\left.\begin{aligned} T_{\beta\alpha} &= P_\beta \bar{V}_\alpha P_\alpha + P_\beta \bar{V}_\beta (JJ^*)^{-1} \sum_\gamma R_\gamma T_{\gamma\alpha} \quad (\beta \neq 0) \\ T_{0\alpha} &= N_{0\alpha} + \sum_{\delta \neq 0} T_\delta R_0 \bar{V}_\delta (JJ^*)^{-1} \sum_\gamma R_\gamma T_{\gamma\alpha} \end{aligned}\right\} \tag{7}$$

where T_δ are the 2-body transition operators in the 3-body space (cf. [1]), and

$$N_{0\alpha} = (H_0 - H_\alpha)P_\alpha + \sum_{\delta \neq 0} T_\delta R_0 (z - H_\alpha + \bar{V}_\delta) P_\alpha \,. \tag{8}$$

The kernel of Eq. (7) is connected without any iteration. Since the kernel minus the identity must simultaneously annihilate all four components of a 4-vector in order for there to exist spurious solutions, there may appear to be some hope that the solution is unique. This hope does not materialize, however, as we have proved that spurious solutions are possible.

Perhaps the most promising aspect of our equations containing channel projection operators is the possibility that some of the P_α operators may be omitted or approximated in an approximation scheme. Work on this subject is in progress and will be the subject of a subsequent paper.

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RESONANCES AND ANALYTIC CONTINUATION

A. Tip

Although the method of obtaining resonances in scattering amplitudes by calculating the positions of complex eigenvalues of a dilated (rotated) non-self adjoint Hamiltonian is a fairly straight forward one, the link between the corresponding resolvent poles and the actual amplitude is still missing for atomic systems. The basic problem is that the Coulomb potentials decay not fast enough to compensate for exponentially growing terms in the amplitude when a continuation to a non-physical sheet is attempted. In the following I want to demonstrate that in a corresponding potential scattering case a continuation can be found that is sufficient for all practical needs.

Thus, we consider a particle scattered from a potential that is in the intersection of $L^1(R^3)$ and the Rollnik class (see [1] for details). The relevant part of the amplitude is given by ($\underline{k}_1$ initial, $\underline{k}_2$ final momentum, $E = k_1^2 = k_2^2$)

$$\Phi(\underline{k}_1 \to \underline{k}_2) = \left(V^{\frac{1}{2}} \left[E + i\varepsilon - H \right]^{-1} V^{\frac{1}{2}} e^{i\underline{k}_1 \cdot x} V^{\frac{1}{2}}, e^{i\underline{k}_2 \cdot x} V^{\frac{1}{2}} \right) \quad (1)$$

where H is the full Hamiltonian and the limit $\varepsilon \to 0$ has to be taken. Now, according to the work of Agmon [2] and Schechter [3]

$$K(E) = \text{uniform} - \lim_{\varepsilon \downarrow 0} V^{\frac{1}{2}} \left[E + i\varepsilon - H \right]^{-1} V^{\frac{1}{2}} \quad (2)$$

exists as a continuous function of $E > 0$ if we rule out positive eigenvalues of H by putting suitable conditions on V. In addition $||K(E)|| < CE^{-\frac{1}{2}}$ for sufficiently large E. Thus, there is a constant $k = k(E_0)$ such that $||K(E)|| < k$ for every $E \in [E_0, \infty) = I$, $E_0 > 0$. But now we are able to approximate the remaining $V^{\frac{1}{2}}$'s

in (1) by exponentially decaying smooth (for instance dilatation analytic) L^2-functions φ while making an arbitrarily small error in the energy interval $[E_0,\infty)$. We end up with an expression for Φ which consists of the sum of an arbitrarily small number and an expression

$$\Psi = \left([E + i\varepsilon - H]^{-1} e^{i\underline{k}\cdot\underline{x}_1}\varphi, e^{i\underline{k}\cdot\underline{x}_1}\varphi\right), E \in I \quad (3)$$

Now we are able to continue Ψ analytically into the second street, provided V is either dilatation analytic or is in a class of potentials discussed by Thomas [4] of not necessarily dilatation analytic potentials where long range tails (Coulomb) are allowed. A similar approach could be followed say for elastic electron-atom amplitudes once one has a corresponding multichannel generalization of the limiting absorption principle. At least, in the energy region below the three-particle break-up threshold this seems to be possible [5].

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NEW, LOCALLY STABLE, SYMMETRIES OF KEPLERIAN SYSTEMS

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We define a physically motivated concept of local stability of an invariance group, and determine new locally stable invariance groups of a Kepler system in the action-angle variable space of Delaunay.

I. Generalities

In their most general form, Hamilton's equations of motion may be written[1]

$$\dot{z}^i - \{W, z^i\} = 0, \; i = 1, 2, \ldots, N. \tag{1}$$

Here $z = (x,y)$ is the vector from the origin to the representative point in the extended phase space PQET, with $x = q,t$ and $y = p, -E$. The coordinates z^i and their derivatives $\dot{z}^i = dz^i/d\omega$ are parameterized by a variable ω. $W(z) = 0$ is the equation of the manifold in phase space which defines the mechanical system. (e.g. $W = H - E$). We have defined the Poisson bracket as

$$\{A,B\} = \sum_r^{N/2} (\partial A/\partial y^r \partial B/\partial x^r - \partial B/\partial y^r \partial A/\partial x^r \tag{2}$$

Let the generator of a continuous group of transformations of the space z be of the most general possible from [2]

$$U = Z^i(z)\partial/\partial z^i = \xi^r \partial/\partial x^r + \pi^r \partial/\partial y^r \tag{3}$$

The group of transformations will leave invariant the equations of motion iff

$$\hat{U} (\dot{z}^i - \{W, z^i\}) \Big| = 0, \; i = 1, 2, \ldots N, \tag{4}$$

Here $\hat{U}$ is the prolongation of U to the space $z, \dot{z}^2$, and the $\Big|$ signifies that the equation is to hold on the subspace for which (1) holds.

$\tilde{U}$ will satisfy (4) iff U satisfies the Lie determining equations:

$$UW\big| = 0, \text{ i.e. } Z^i(z)\, W_i(z)\big| = 0 \tag{5a}$$

$$\{W, \xi^r\} - U\, \partial W/\partial y^r\big| = 0 \tag{5b}$$

$$\{W, \pi^r\} + U\, \partial W/\partial x^r\big| = 0 \tag{5c}$$

These equations have a non-denumerably infinite number of linearly independent solutions U_α. Subsets of these close under commutation yielding various R parameter Lie algebras, R > 1;

$$[U_\alpha, U_\beta] = C^\gamma_{\alpha\beta}\, U_\gamma, \quad \alpha, \beta, \gamma = 1, 2, \ldots, R. \tag{6}$$

Several different sets of generators may have the same commutation relations and integrate to different realizations of the same abstract Lie group.

For reasons of stability some U_α may be expected to be of more physical importance than others. We make the following definition:

Let M be a differentiable manifold defined by W (z) = 0. Let

$$UW = 0 \qquad \text{on } W = 0 \tag{7a}$$

Then U, and the group generated by it, will be said to be locally stable about M if, for arbitrary infinitesimal δz,

$$Z^i(z + \delta z)\; W_i(z + \delta z) = 0, \text{ when } W(z) = 0. \tag{7b}$$

For this to be true it is sufficient that for all j

$$\partial/\partial z^i\,(UW)\big| = 0. \tag{8}$$

If and only if U is locally stable about M will the group generated by U leave M invariant when the coordinates of M are uncertain to within the margin δz, as must be the case for all physically realizable systems. Any finite transformation of a locally stable group carries two points whose separation $|\delta z|$ is infinitesimal into

two points whose separation is infinitesimal as long as these points are infinitesimally close to M. Local stability is thus a natural generalization of the concept of neutral stability.[3]

Now U will be the generator of a continuous group of canonical transformations in PQET if

$$U = \{I(z)\ \cdot\} \quad , \quad -\infty \leq z^i \leq \infty \quad , \tag{9}$$

where I(z) is an arbitrary analytic function. We will say that U is the generator of an M-canonical transformation if, for all i,

$$U\, z^i|_M = \{I,\ z^i\}\,|_M \tag{10}$$

THEOREM:[4]

The generator of a canonical or M-canonical transformation that leaves invariant Hamilton's equations of motion on a manifold M is locally stable about M.

The proof simply involves writing out equations (5) in full, adding to, and subtracting from them, the LHS of (8), and using (9) or (10).

Constants of the motion I(z) are associated with canonical and M-canonical transformations as follows:

i) If $UW \equiv 0$, the $\partial / \partial z^i (UW) \equiv 0$ for all i. Hence if $U = \{I\ \}$, then
$$\dot{I} = \{W, I\} = - UW \equiv 0.$$

ii) If $UW|_M = 0$, and $\partial/\partial z^i (UW)|_M = 0$ for all i, and if $Uz^i|_M = \{I, z^i\}|_M$ for all i, then $\dot{I}|_M = \{W,I\}|_M = -UW|_M = 0$.

when $W = H - E$ with $H = H(q,p)$ one has $dw = dt$, and $\{H - E, I\}_{PQET} = \{H, I\}_{PQ} + \partial I/\partial t$.

Thus if U is the generator of a canonical or M-canonical transformation that is a locally stable invariance transformation of the manifold $W(z) = 0$, then I(z) is a constant of the motion. If $I = I(q, P, -E)$, I is a <u>first integral</u>, otherwise, if $W = H - E$, I is a

time-dependent constant of the motion. When I is a first integral, $U = \{I \cdot\}$ or $\{I \cdot\}|_M$ is the generator of a degeneracy group. In the general case the invariance operators U are generators of a dynamical group.

II. Degeneracy Groups of Bound Kepler Systems In Delaunay's Phase Space

The dependence of the Kepler Hamiltonian on the usual action variables J_r, J_θ, J_ψ is given by [5]

$$H = -1/2\ Z^2\ (J_r + J_\theta + J_\psi)^{-2}, \tag{11}$$

the corresponding angle variables being α_r, α_θ, α_ψ. Because of the multivaluedness introduced in the transformation from ordinary phase space to the space of the variables J, α, the transformation is not a homeomorphism, and we can not expect that the equations of motion admit the same abstract Lie groups on both spaces. The standard Delaunay variables are [5]

$$\begin{aligned} x^1 &= \alpha_\psi - \alpha_\theta \quad , \quad y^1 = J_\psi \\ x^2 &= \alpha_\theta - \alpha_r \quad , \quad y^2 = J_\psi + J_\theta \\ x^3 &= \alpha_r \quad , \quad J = J_\psi + J_\theta + J_r \end{aligned} \tag{12}$$

Let

$$x^4 = t,\ y^4 = -E, \text{ and } y^3 = J - J_o \tag{13}$$

where $E = -1/2Z^2(J_o)^{-2}$. Then

$$y^3|_M = 0, \quad M: \ H - E = 0 \tag{14}$$

the variables x^1, x^2, y^1, y^2, y^4 are constants of the motion y^1 fixes the z-component of the angular momentum and y^2 fixes the total angular momentum. x^1, x^2 then fix the orientation of the orbit with respect to an axis system. J (J_o) determines the length of its major axis; J and y^2 together determine its eccentricity. [6]

For any analytic function f $(x^1, x^2, y^1, y^2, y^4)$,

$$U = \{f \cdot\} \tag{15}$$

is the generator of a one-parameter degeneracy group. Also from the theorem it follows that if

$$g_{k\ell} = (y^3)^k (x^3)^\ell, \quad k \geq 2, \quad \ell \geq 0,$$

then

$$U = \{g_{k\ell} \cdot\} \tag{16}$$

also generates a degeneracy group canonical on M. It follows that for any analytic function $F(x^1, x^2, y^1, y^2, g_{k\ell}, y^4)$,

$$U = \{F \cdot\} \tag{17}$$

also generates such a group.

In Table 1 we display all linearly independent U's of this form (17) which satisfy the two criteria:

i) The corresponding F contains no terms of total order greater than 3.

ii) The generator U is a member of Lie algebra of dimension two or greater.

Tables 2, 3 summarize the commutation relations of these generators.

The generators in these tables may be considered to be "kernels" for other realizations with the same group properties: Denoting the generators in the tables by V_α one may define generators

$$V_{\alpha F} = (\exp a\, U_F)\, V_\alpha\, (\exp - aU_F), \text{ a a parameter.}$$

The $V_{\alpha F}$ have the same commutation relations as the V_α, and are generators of degeneracy groups.

The largest group we find has as "kernel" the direct product of the 10 parameter symplectic group in x^1, x^2, y^1, y^2, and a one-parameter group with generator $\{g_{21} \cdot\}$. Note that none of the groups contain SO(4).

Acknowledgement

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TABLE I

$X_i = \partial_{X_i} = \{Y_i \cdot\}$

$Y_i = \partial_{Y_i} = -\{X_i \cdot\}$

$X_{ij} = Y_i\partial_{X_j} + Y_j\partial_{X_i} = \{Y_iY_j \cdot\}$

$Y_{ij} = X_i\partial_{Y_j} + X_j\partial_{Y_i} = -\{X_iX_j \cdot\}$

$Z_{ij} = X_i\partial_{X_j} - Y_j\partial_{Y_i} = \{X_iY_j \cdot\}$

$P_i = X \cdot Y\partial_{Y_i} - X_iA = -\{X \cdot Y\ X_i \cdot\}$

$Q_i = X \cdot Y\partial_{X_i} + Y_iA = \{X \cdot Y\ Y_i \cdot\}$

GENERATORS

TABLE 2

	X_i	Y_i	X_{ij}	Y_{ij}	Z_{ij}	P_i	Q_i
X_i	0	0	0	X_i	X_i	Z_{ij}	X_{ij}
Y_i		0	Y_i	0	Y_i	Y_{ij}	Z_{ij}
X_{ij}			0	Z_{ij}	X_{ij}	•	•
Y_{ij}				0	Y_{ij}	•	•
Z_{ij}					Z_{ij}	P_i	Q_i
P_i						0	•
Q_i							0

(• means no closure.)

SUMMARY OF COMMUTATION RELATIONS

TABLE 3

$X_i \bullet Y_j$	4	$Y_i \bullet Y_{jk}$	5
$X_i \bullet X_{jk}$	5	$Y_i \bullet Z_{jk}$	6
$X_i \bullet Y_{jk}$	5	$Y_i \bullet Q_j \bullet Z_{kl}$	8
$X_i \bullet Z_{jk}$	6	$X_{ij} \bullet Z_{kl}$	7
$X_i \bullet P_j \bullet Z_{kl}$	8	$Y_{ij} \bullet Z_{kl}$	7
$Y_i \bullet X_{jk}$	5	$X_{ij} \bullet Y_{kl} \bullet Z_{mn}$	10

DIMENSIONS OF CLOSED ALGEBRAS

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OPTIMIZED APPROXIMATE SOLUTIONS TO THE TIME DEPENDENT SCHRÖDINGER EQUATION

A.B. Weglein

For the time dependent Schrödinger equation

$$G\psi = 0$$

$$G = H - i\frac{\partial}{\partial t}$$

a trial solution, ψ_{tr}, can be sought in terms of paramaters. The trial solution will satisfy

$$G\psi_{tr} = \psi_1$$

Define levels of optimization:

Level (A) $|\psi_1|^2$ be a minimum at every $\vec{r}$ and t

Level (B) $\int|\psi_1|^2\, d\vec{r}$ be a minimum at every t

Level (C) $\int|\psi_1|^2\, d\vec{r}\, dt$ be a minimum

Unfortunately, the forms of trial solutions (with time dependent parameters) used in typical applications are not sufficiently flexible to achieve level A or B optimization. Level C optimization can be realized.

For a trial solution, ψ_{tr}, that depends on N complex parameters, α_i, and M real parameters, λ_i, define momenta conjugate to these parameters

$$P_{\alpha_i} = \frac{\partial D}{\partial \dot{\alpha}_i} \quad (i = 1,2,\ldots N)$$

$$P_{\lambda_i} = \frac{\partial D}{\partial \dot{\lambda}_i} \quad (i = 1,2,\ldots M)$$

where $D(t) = \int d\vec{r}|\psi_1|^2$. A pseudo-Hamiltonian K is also defined

$$K = \sum_{j=1}^{N} (\dot{\alpha}_j P_{\alpha_j} + \dot{\alpha}_j^* P_{\alpha_j}^*) + \sum_{i=1}^{N} \dot{\lambda}_i P_{\lambda_i} - D$$

and Hamilton's equations are then

$$\dot{\alpha}_j = \frac{\partial K}{\partial P_{\alpha_j}} \quad (j = 1,2,\ldots N)$$

$$\dot{P}_{\alpha_j} = -\frac{\partial K}{\partial \alpha_j} = \frac{\partial D}{\partial \alpha_j} \quad (j = 1,2,\ldots N)$$

$$\dot{\lambda}_i = \frac{\partial K}{\partial P_{\alpha_i}} \quad (i - 1,2,\ldots M)$$

$$\dot{P}_{\lambda_i} = -\frac{\partial K}{\partial \lambda_i} = \frac{\partial D}{\partial \lambda_i} \quad (i = 1,2,\ldots M)$$

The simultaneous solution of these equations leads to a level C optimized ψ_{tr}. If the parameters are chosen to be the *expansion coefficients* of a truncated eigenfunction expansion, the P_α give a single average contribution from the excluded part of Hilbert space[1]. For a simple example of a real parameter internal to the expansion functions, the P_λ turn out to represent a time delay correction[1].

This technique for calculating parameters in trial solutions would be: (1) useful and convenient for internal parameters and (2) useful for expansion coefficients where the important states are either too numerous or not precisely known.

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ERROR ESTIMATES IN VARIATIONAL SCATTERING CALCULATIONS

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The variational method [1-3] is one of the most powerful and widely used methods for the approximate determination of scattering phaseshifts. In the most commonly used version of the method [2] neither the sign nor magnitude of the error that is made are generally known, though there are exceptions to this. Kato [3] was the first to propose a method of determining bounds on the error in such variational calculations. This bound is given in terms of the so-called variance integral (equation (8) below) and approximations to certain eigenvalues of an auxiliary eigenvalue problem.

We propose a somewhat different expression for the bounds on the error: Initially we shall consider potential scattering of a given partial wave, that is we are seeking a variational approximation to the solution of

$$Lu(r) = u'' + [k^2 - V(r)]u = 0 \tag{1}$$

where the radial wave u(r) satisfies the 'boundary' conditions

$$u(r=0) = 0 \text{ and } u(r\to\infty) = A(\eta)\sin(kr - \ell\,\frac{\pi}{2} + \eta), \tag{2}$$

$A(\eta)$ being an arbitrary normalization constant, most commonly taken to be $\sec\eta$.

If $u_T(r)$ is an approximation to u(r) satisfying the same conditions (2), but with the unknown η replaced by some trial value η_T, then the variational principle sates:

$$I[u_T,u_T] = kA(\eta)\ A(\eta_T)\ \sin(\eta-\eta_T) + I[u_T - u, u_T - u] \tag{3}$$

where

$$I[v,w] = \int_0^\infty vLw\ dr. \tag{4}$$

Neglect of the 'second order' error term $I[u_T - u,\ u_T - u]$ in (3) allows the determination of a stationary approximation to η in

terms of u_T. Since $Lu = 0$, it follows that the error

$$|I[u_T - u,\ u_T - u]| \leq |u_T - u|_M \int_0^\infty |Lu_T| dr = |u_T - u|_M \mathcal{L}_1 \qquad (5)$$

the subscript M referring to the maximum value of the expression in $0 \leq r < \infty$. Using the Lippman-Schwinger equation it is straight forward to show that

$$|u_T - u|_M \leq |f|_M/(1 - g_M) \qquad (6)$$

where $f(r) = \int_0^\infty G(r,r')\ Lu_T(r')dr'$, G being the appropriate Green's function, provided that the effective potential V(r) satisfies the condition

$$g_M = \text{Max of} \int_0^\infty |G(r,r')\ V(r')|\ dr' < 1\ . \qquad (7)$$

We note also that if w(r) is any weight function such that the indicated integrals exist, then

$$\mathcal{L}_1^2 \leq \mathcal{L}_2^2 = \int_0^\infty |w|^{-2}\ dr \int_0^\infty |w L u_T|^2\ dr = \int_0^\infty |w|^{-2}\ dr \cdot U, \qquad (8)$$

U being the variance integral. We illustrate our results by considering s-wave scattering by an exponential potential $V(r) = -2e^{-2r}$ (a.u.) using $w = e^{\gamma r}$ and the trial function,

$$u_T(r) = \sin kr + \tan\eta_T\ \cos kr\ (1 - e^{-\alpha r}) + \sum_{i=1}^{N} a_i r^i\ e^{-pr}\ . \qquad (9)$$

The variational parameters $\alpha, p, \gamma, \tan\eta_T, a_i$ are chosen such that the error bounds, $f_M\ \mathcal{L}_1/(1 - g_M) \leq \mathcal{L}_1^2/k(1 - g_M) \leq \mathcal{L}_2^2/k(1 - g_M)$, are minimized. The results are given in Table 1 below, where we give also the first order bounds $\tan\eta_T \pm \mathcal{L}_2/k(1 - g_M)$ derived previously by Bardsley et al [4]. (Note that $\tan\eta_2 = \tan\eta_T + \frac{1}{k} I[u_T, u_T]$) The order of magnitude improvement over their values is clearly evident.

The present results generalize in a straightforward way to the case of scattering by a compound system, but (without modification) they become computationally intractable because of the complex structure of the Green's function in that case.

Table a. Variational bounds for $V = -2e^{-2r}$(a.u.), $\ell = 0$, $N = 2$.

	k = .02	k = .5
$\tan\eta$ (exact)	.01474138	.26107327
$\tan\eta_T$	.01475087	.26106443
$\tan\eta_2$	.01474138	.26107324
$\tan\eta_T + \frac{f_2}{k(1-g_m)}$	.01967730	.26536480
$\tan\eta_T - \frac{f_2}{k(1-g_m)}$	.00982444	.25676407
$\tan\eta_2 + \frac{f_2^2}{k^2(1-g_m)}$	.01475352	.26108249
$\tan\eta_2 - \frac{f_2^2}{k^2(1-g_m)}$	.01472818	.26106400
$\tan\eta_2 + \frac{f_m f_1}{k(1-g_m)}$	.01474272	.26107759
$\tan\eta_2 - \frac{f_m f_1}{k(1-g_m)}$	.01474004	.26106889

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ON THE SUMMATION OF PARTIAL WAVE EXPANSIONS IN POTENTIAL SCATTERING

F.F.Grinstein and C.R.Garibotti

A usual method for the calculation of differential cross-sections is that based on the partial wave expansion of the scattering amplitude (PWESA). For two body potential scattering, the number of terms with an important contribution to that series is given by the semiclassical relation.

$$N_{max} \sim kr_o$$

where k is the magnitude of the wave vector and r_o is the effective range of the potential. Thus, this method is of great value when relatively low values of r_o, of the energy and of the reduced mass of the system, are involved. Otherwise, the convergence of the series is slow and a considerable number of phase-shifts must be calculated, in order to obtain accurate values for the amplitude. Typical of these situations, are atomic and molecular collision processes, where long range interactions are present, and nuclear systems described by short range potentials, in the intermediate energy range.

Several alternative methods of calculation are valid for some of these cases, such as the semiclassical and distorted wave approximations. However, an interesting global approach is to keep the original PWESA, and to find adequate mathematical methods to resume efficiently the information contained in the terms of series.

Such methods are available within the framework of Padé-type approximations, and some of them have been proposed for that purpose [1-7]. Here, we review in particular, the work done on these lines by using Punctual Padé Approximants (PPA). This approach is related to a sequence transformation method introduced by Shanks [8], and has the attractive feature, from the numerical point of view, of counting on algorithms which allow for the recurrent calculation of successive approximations [6].

For long range potentials, having the asymptotic behaviour

$$V(r) \underset{r \to \infty}{\sim} V_o\, r^{-\alpha-2} \quad , \quad \alpha \geq -1$$

where α is an integer, the convergence of the sequences $[n,n+m]$ of PPA to the PWESA was proved for fixed $m > 0$ and $n \to \infty$, i.e., for the non trivial rows of the PPA table [5]. This includes, in particular, the case $\alpha = -1$ (for $n \geq 2$ and $\theta > 0$), where the PWESA is divergent for all values of the scattering angle θ, and $\alpha = 0$, $\theta = \pi$ (for $n \geq 1$), where it is oscillating, covering all of the cases for which the amplitude has *finite* meaningful values in the physical interval $-1 \leq \cos\theta \leq 1$, where the convergence of the PWESA is, in principle, restricted. Moreover, the asymptotic rate of convergence of the PPA sequences considered was shown to increase rapidly with n. The sequence of partial wave sums, i.e., the first row of the table, turned out to be, consequently, the poorest with regards to convergence. Furthermore, a numerical study of the approach, applied to typical situations involving long range potentials, showed its importance from the practical point of view [6].

The same general features regarding the convergence of the rows of the PPA table were proven [7] in case of short range potentials with the behaviour

$$V(r) \underset{r \to \infty}{\sim} V_o r^{-s-1} \exp(-ar), \; s \text{ integer}, \; a > 0$$

The proof is restricted to the Lehmann ellipse in the complex cos θ plane, where the PWESA converges. However, owing to the rational nature of the PPA and their good behaviour within this domain, they can be expected to be a valuable means for the approximate analytical continuation of the scattering amplitude in the cos θ plane, at least, in applications involving this type of potentials. This possibility deserves further study.

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APPLICATION OF THE CLOSE-COUPLING METHOD TO EXCITATION OF ELECTRONIC STATES AND DISSOCIATION OF H_2 BY ELECTRON IMPACT

Sunggi Chung and Chun C. Lin

If an excitation of electronic states is the primary interest in an electron-molecule collision, the molecular vibration and rotation may be treated separately. We assume this has been done. (A fuller account of this presentation will be published [1].) The targe molecule is charaterized by $(n\lambda)$, λ being the angular mementum along the molecular axis, and the scattered electron by (ℓm). We adopt the representation in which $\Lambda = \lambda+m$ is diagonal, and use the molecule-fixed frame of reference. A channel is defined as $\mu = (n\lambda\ell)$. We have the scattering equation

$$[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2]F_\mu(r) = \sum_\mu [U_{\mu\mu'}(r) + W_{\mu\mu'}(r)]F_{\mu'}(r) + (\text{orthogonality terms}). \quad (1)$$

This set of integro-differential equations may be solved, for example, by the noniterative integral-equation method (NIEM) [2]. The direct coupling potentials may be written as (apart from the part due to the nuclear charge)

$$V^e_{\mu\mu'}(r) = \sum_{K=|\ell-\ell'|}^{\ell+\ell'} c^K(\ell'\Lambda-\lambda',\ell\Lambda-\lambda)\, y_K(\phi_j,\phi'_j|r), \quad (2)$$

$$y_K(\phi_j,\phi'_j|r) = (-1)^{\lambda'_j-\lambda_j}[\frac{4\pi}{2K+1}]^{1/2} \times [\{r^{-K-1}\int_o^r r'^K r'^2 dr' + r^K \int_o^\infty r'^{-K-1} r'^2 dr'\} \times \{\int d\hat{r}'\, \phi^*_j(n_j\lambda_j|r')Y_{K,\lambda_i-\lambda'_j}(\hat{r}')\phi'_j(n'_j\lambda'_j|r')\}], \quad (3)$$

where ϕ_j, ϕ_j' are molecular-orbital (MO) wave functions. We express MO as linear combinations of atomic orbitals (LCAO) and the atomic orbitals by the Gaussian-type orbitals (GTO). We choose the coordinate system with the origin at the center of diatomic molecule so that two nuclei are at (0,0,R/2) and (0,0,-R/2) respectively and the z-axis along $\vec{OA}$. Then

$$\phi(\sigma_g) = \sum_i c_i \{G(a_i,A) + G(a_i,B)\} + \sum_j c_j \{(r\cos\theta - \frac{R}{2})\, G(a_j A) - (r\cos\theta + \frac{R}{2})\, G(a_j,B)\} \quad (4)$$

etc., with

$$G(a,A) = \exp[-a(R^2/4 + r^2 + Rr\cos\theta)],$$
$$G(a,B) = \exp[-a(R^2/4 + r^2 - Rr\cos\theta)]. \quad (5)$$

With the substitution of Eq. (4), the θ-integral of the last line in Eq. (3) always has the form (ϕ-integral is trivial),

$$\int_o^\pi e^{x\cos\theta} \cos^n\theta \sin\theta d\theta = P_n(x)e^{-x} + Q_n(x)e^{+x}, \quad (6)$$

$$P_n(x) = (-1)^{n+1} \sum_{m=o}^{n} \frac{n!}{(n-m)!\, x^{m+1}}$$
$$Q_n(x) = (-1)^n P_n(-x) . \quad (7)$$

The computer program is divided into three parts: The first program computes Eq. (7) and "outputs" onto a tape the coefficients P_n and Q_n of all relevant orbital-combinations (ϕ_j,ϕ_j') for sufficiently large values of K. The second program numerically integrates by Simpson's rule Eq. (3) and copies onto a second tape $y_K(\phi_j,\phi_j'|r_m)$, m = 1,2,... . At this point the quadrature scheme (step-size, etc.) to be used in the scattering equations are committed to. The third program assembles Eq. (2) and the part due to the nuclear charge to form $U_{\mu\mu'}(r_m)$, m = 1,2,... . These potentials are copied out onto a third tape by blocks as

follows: (1) $m = 1,2,\ldots M_1$; (2) $m = M_1 + 1,\ldots M_2$; etc. But all combinations of μ,μ' are included in each block. The scattering-equation program copies in one block at a time as needed. The exchange potentials are treated in an analogous manner.

We used the computational procedure described above to calculate cross sections of the $b^3\Sigma_u^+$, $a^3\Sigma_g^+$, $e^3\Sigma_u^+$, $c^3\Pi_u$, and $B^1\Sigma_u^+$ states.

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THE POLARIZED-ORBITAL APPROXIMATION IN ELECTRON AND POSITRON SCATTERING FROM ATOMS

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The polarized orbital approximation has recently been applied to positron scattering from helium and neon with very good results [1,2,3]. In our version of the approximation all multipole moments of the positron-atom interaction have been included, either by means of an explicit calculation or, in the case of the higher multipoles, via an extrapolation procedure [2,3]. For positron-atom scattering the static and polarization potentials have opposite signs. Thus to obtain an accurate potential at intermediate distances all such moments must be included.

The resulting integro-differential equations for the polarized-orbitals were solved via an iterative procedure. However in order to obtain convergence for the dominant dipole polarized orbital it was necessary to use a variation of the iterative method which involved a dynamic acceleration parameter [2].

The calculation of positron scattering provides a severe test of the theory used since, in addition to the usual scattering phenomena annihilation processes also occur. In the case of positron scattering from argon our results for the momentum transfer cross section and the effective number of annihilation electrons (Z_{eff}) have the correct behavior (Canter et al [4]) though the agreement between our elastic cross section results and recent experimental data is less good than in the case of helium and neon. Another quantity is the angular correlation between the photons produced during annihilation. We present our results in fig. 1 along with the measurements of Briscoe et al [5].

In the case of electron scattering from noble gases we replace the exchange kernel by a local potential. For scattering from helium we use the modified semiclassical exchange approximation of

Bransden and Noble [6]. For neon and argon we found that a combination of the semiclassical exchange approximation of Furness and McCarthy [7] for the inner region and the free-electron-gas exchange approximation of Hara [8] for the outer region yielded the best results. The static and polarization potentials were the same as the ones used for positron scattering.

Our results for the elastic scattering of electrons from helium and neon agree very closely with the experimental data. In the case of scattering from argon the agreement is less good. In fig. 2 we present the data for neon.

We have shown by explicit calculation that the polarized orbital approximation, when suitably applied, is capable of yielding very accurate results for electron and positron scattering from atoms. This is true not only for gross features like cross sections but also for phase shifts and annihilation processes.

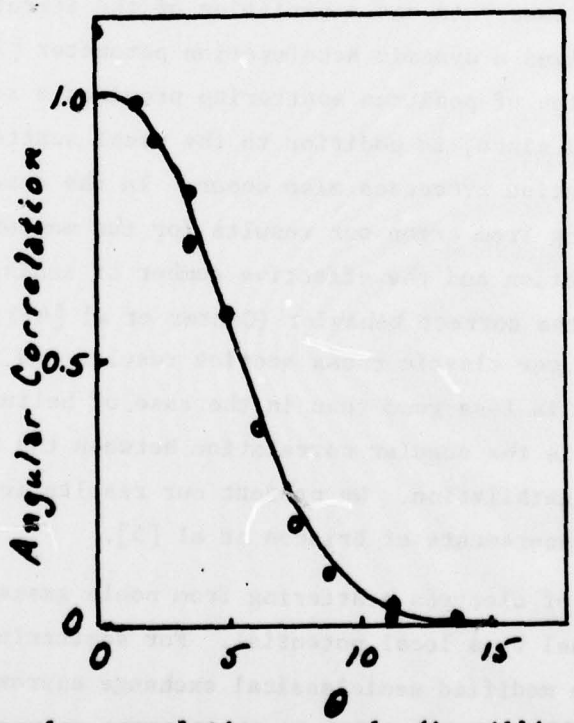

Fig.1. Angular correlation vs angle (in milliradians): ___, present work, o experimental points [5].

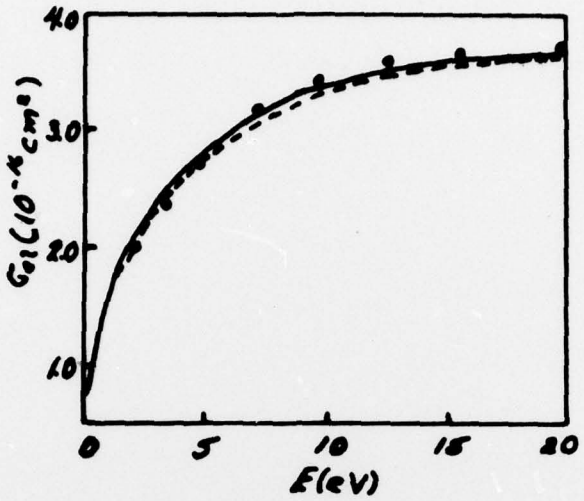

Fig. 2. Elastic cross sections vs energy: ____, present work, _ _ _, experiment [9] ; o experimental points [10].

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The Conference on Mathematical and Computational Aspects of Atomic Scattering Theory was held June 7-9, 1978 at the University of Western Ontario. About 50 scientists participated in the meeting, which was organized by T.M. Luke and J. Nuttall of the Theoretical Physics Group of the University of Western Ontario. The aim of the conference was to bring together people who approach the problem of Atomic Scattering Theory from varying viewpoints, which range from the rigorous mathematical to the purely computational.

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